

Synthesis of biaryl-based carbazoles via C-H functionalization and exploration of their anticancer activities

Ramandeep Kaur,^a Haritha Dilip,^b Sivapriya Kirubakaran,^{*b} Srinivasarao Arulananda Babu^{*a}

^a Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali Knowledge City, Sector 81, SAS Nagar, Mohali, Manauli P.O., Punjab, 140306, India. E-mail: sababu@iisermohali.ac.in

^b Department of Chemistry, Indian Institute of Technology Gandhinagar, Palaj Village, Gandhinagar, Gujarat, 382055, India. E-mail: priyak@iitgn.ac.in

Contents

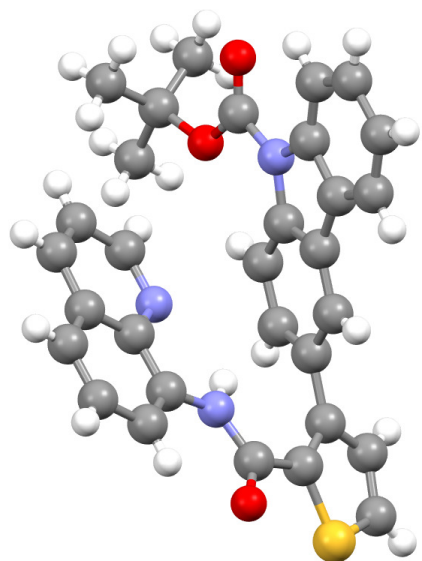
X-ray structure and brief X-ray data of compound = p2-3

Proton and carbon NMR of compounds = p4-543

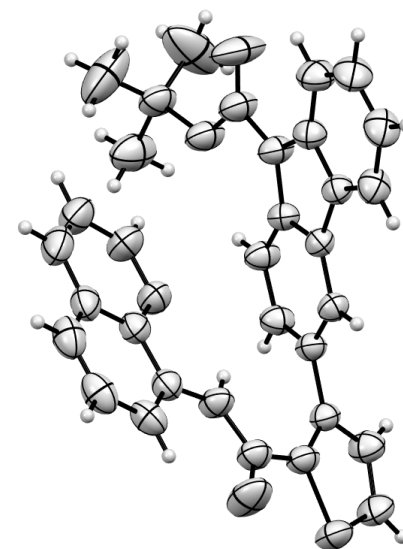
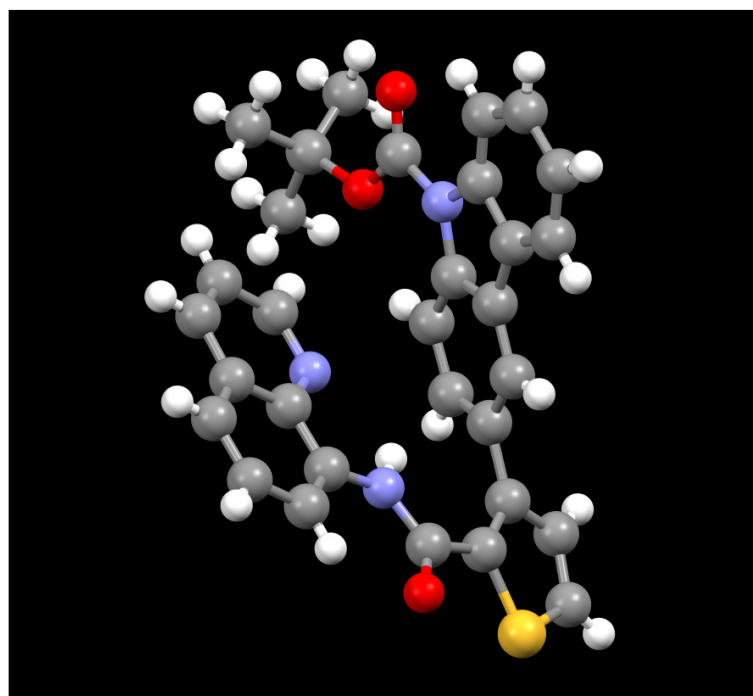
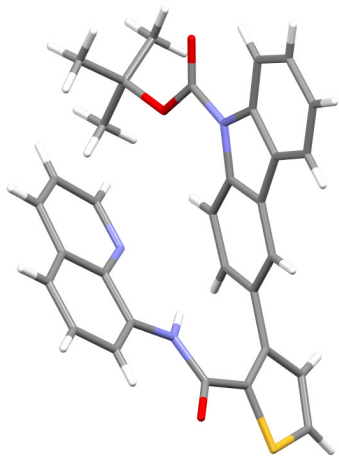
UV-Vis absorption spectra of compounds, λ_{max} (absorption) and fluorescence emission of representative biaryl-based carbazole = p544-560

Figures of biological evaluation of the synthesized compounds = p561-567

X-ray structure of compound

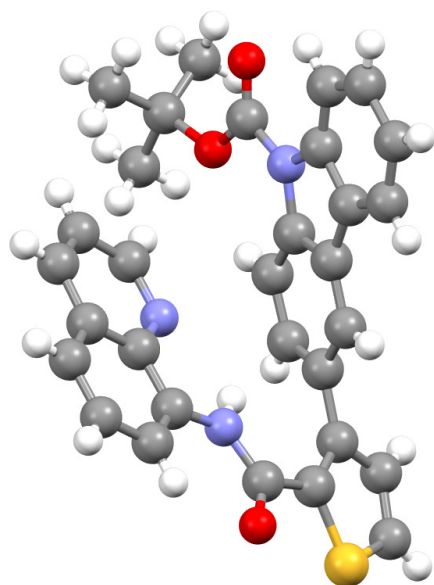


CCDC 2378236



ORTEP diagram
Ellipsoid probability = 50%

X-ray structure and
brief crystal data of compound
CCDC 2378236



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rd319

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: rd319

Bond precision: C-C = 0.0035 Å Wavelength=0.71073

Cell: a=8.8101 (9) b=12.3193 (11) c=13.1329 (10)
 alpha=92.965 (7) beta=109.135 (8) gamma=96.379 (8)

Temperature: 273 K

	Calculated	Reported
Volume	1332.4 (2)	1332.4 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H25 N3 O3 S	C31 H25 N3 O3 S
Sum formula	C31 H25 N3 O3 S	C31 H27 N3 O3 S
Mr	519.60	521.61
Dx, g cm ⁻³	1.295	1.300
Z	2	2
Mu (mm ⁻¹)	0.159	0.159
F000	544.0	548.0
F000'	544.47	
h, k, lmax	13, 18, 19	12, 17, 19
Nref	9819	8214
Tmin, Tmax	0.953, 0.969	0.876, 1.000
Tmin'	0.953	

Correction method= # Reported T Limits: Tmin=0.876 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.837 Theta(max)= 32.709

R(reflections)= 0.0599 (4088)

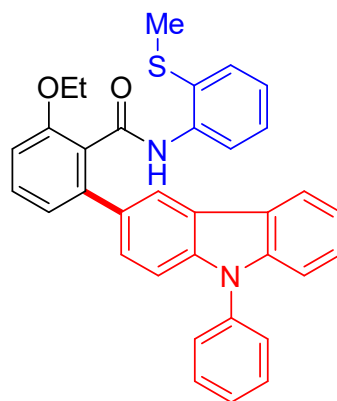
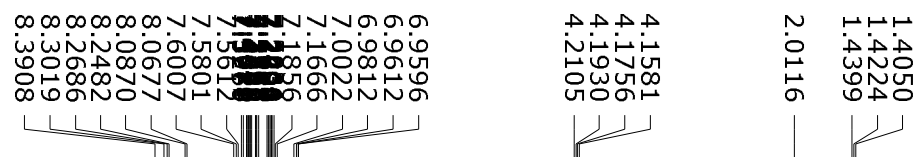
wR2(reflections)=
0.1980 (8214)

S = 1.022

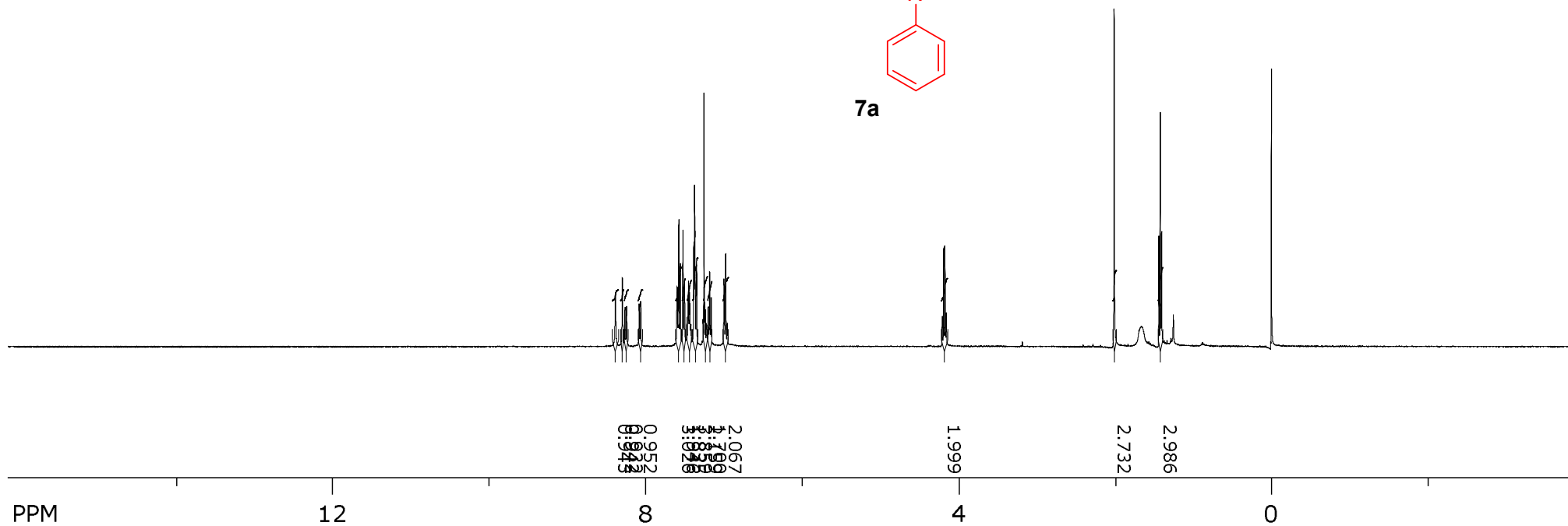
Npar= 346

SpinWorks 4: RD 835

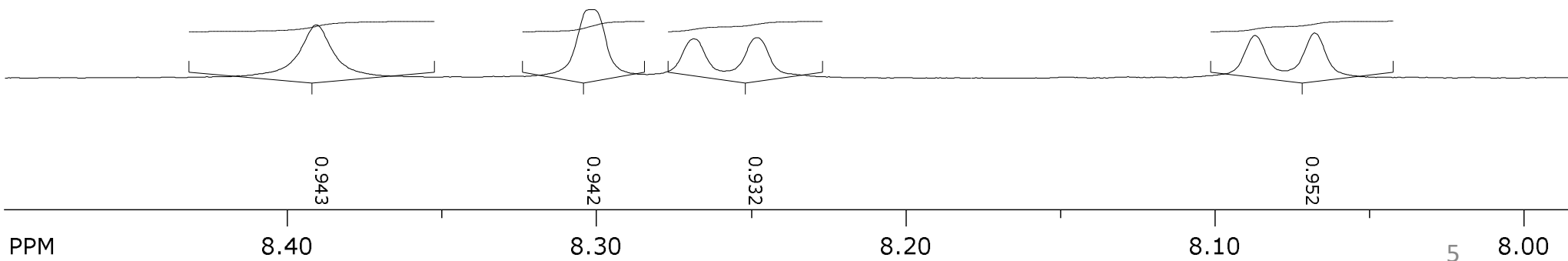
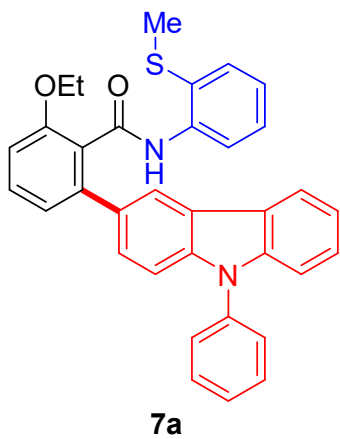
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7a



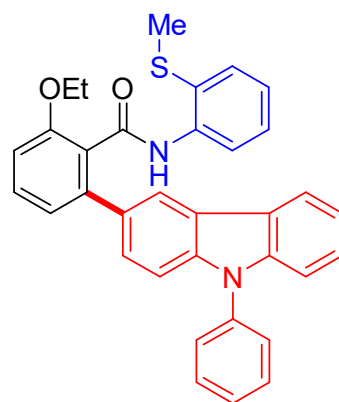
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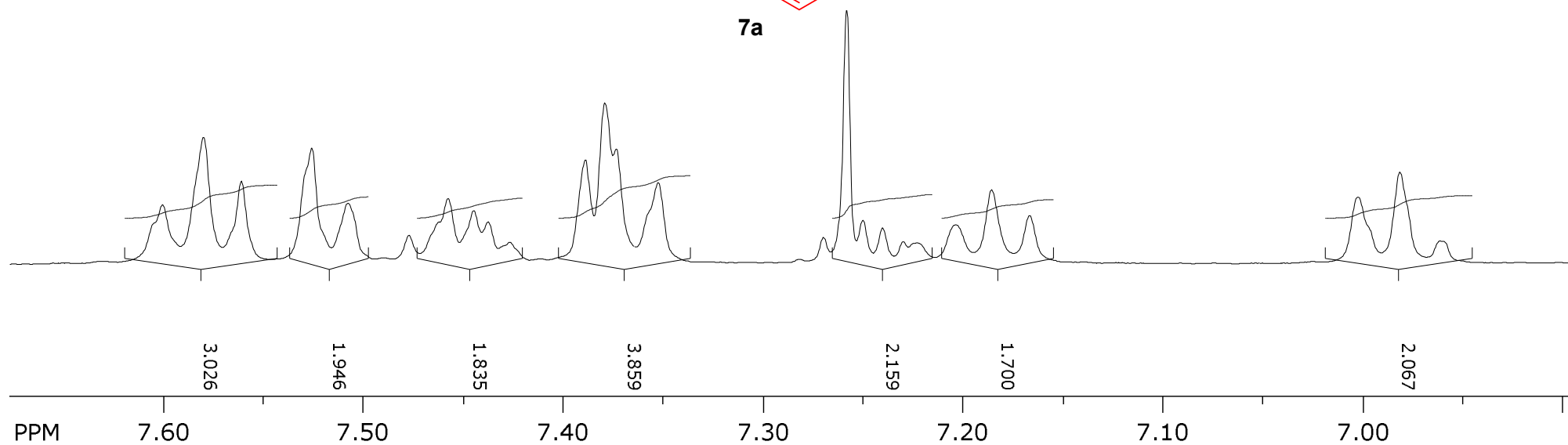
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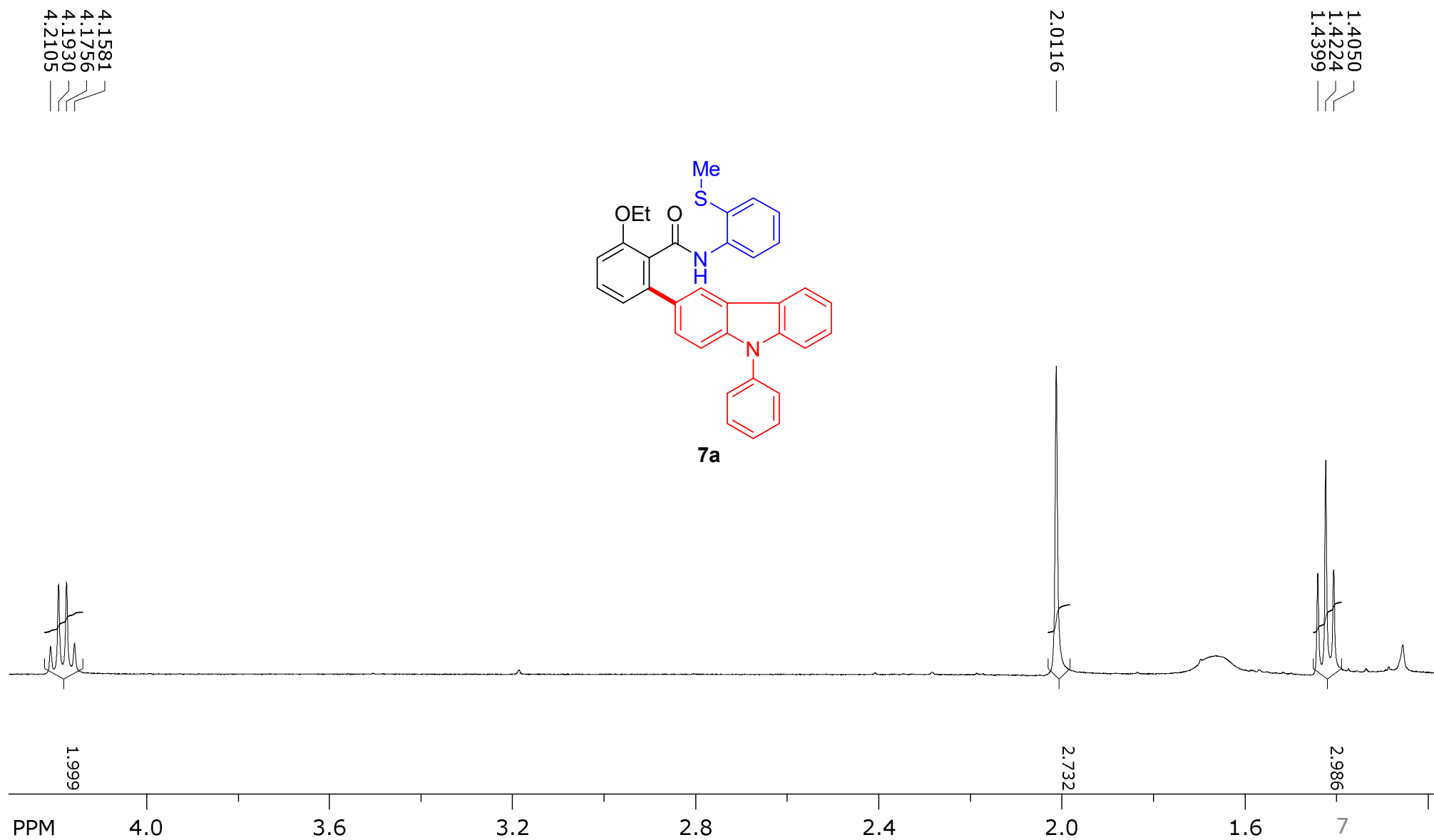
7.6007	7.5612	7.5260	7.5078	7.4773	7.4621	7.4577	7.4448	7.4376	7.4268	7.3890	7.3792	7.3735	7.3525	7.2698	7.2581	7.2500	7.2402	7.2298	7.2230	7.2034	7.1856	7.1666	7.0022	6.9812	6.9612	6.9596	
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



7a



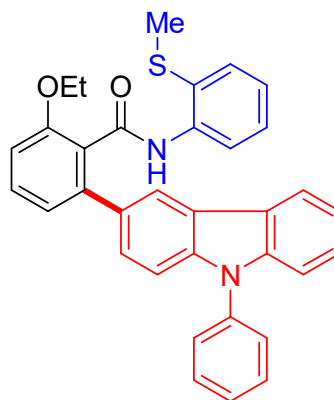
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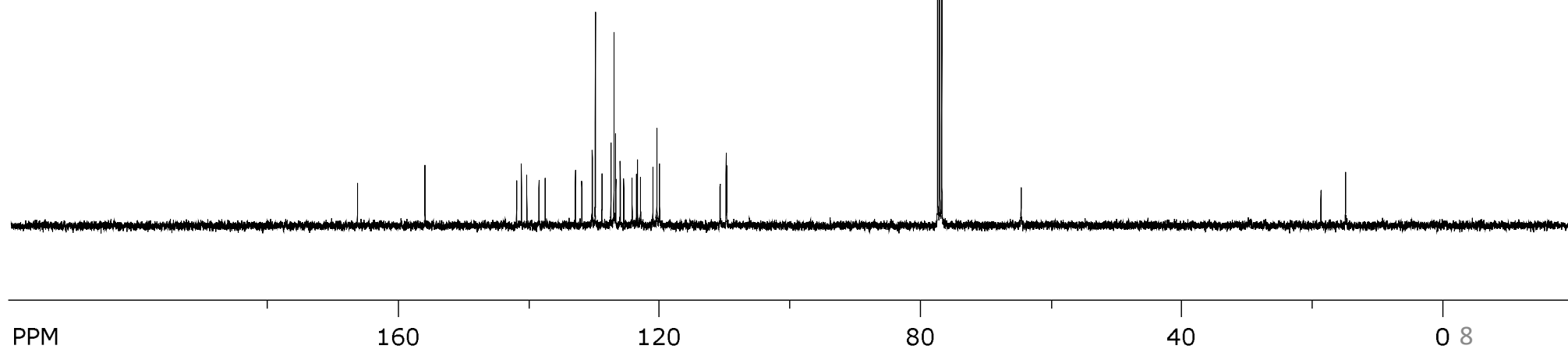
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C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

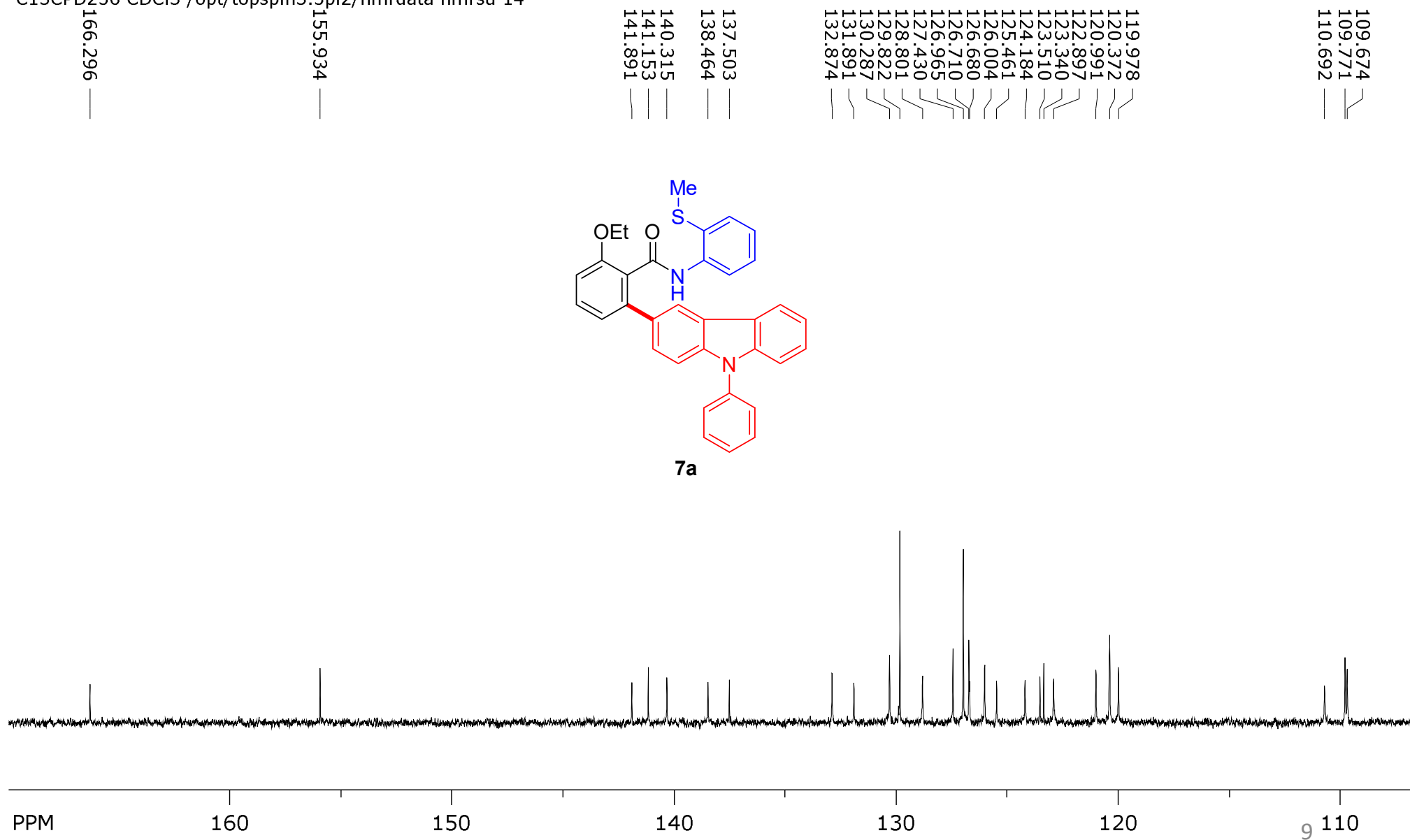
166.296
155.934
141.891
141.153
140.315
138.464
137.503
132.874
131.891
130.287
129.822
128.801
128.099
127.999
123.540
122.897
120.991
120.372
119.978
110.692
109.771
109.674
77.338
77.020
76.703
64.536
18.559
14.794



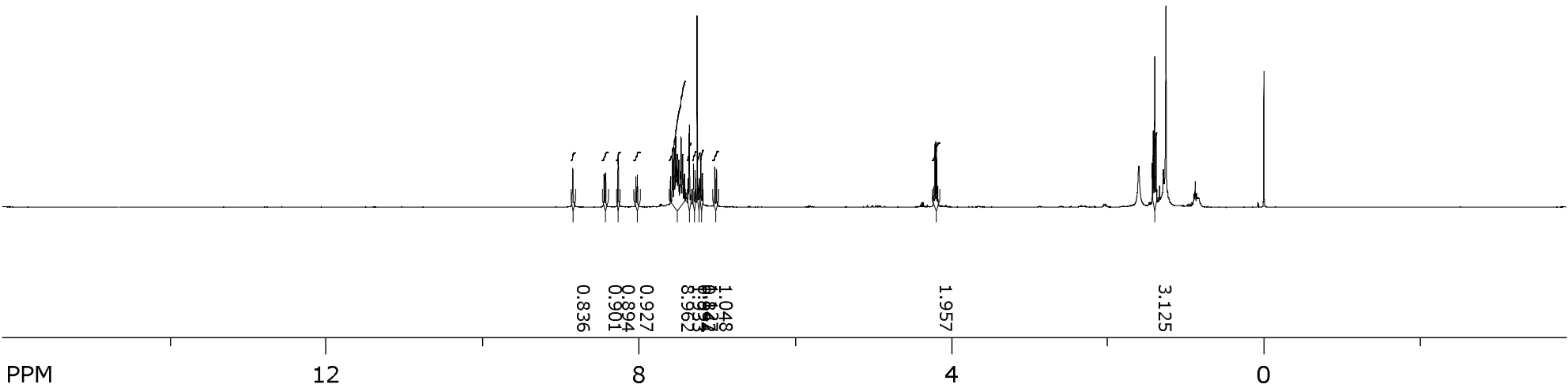
7a



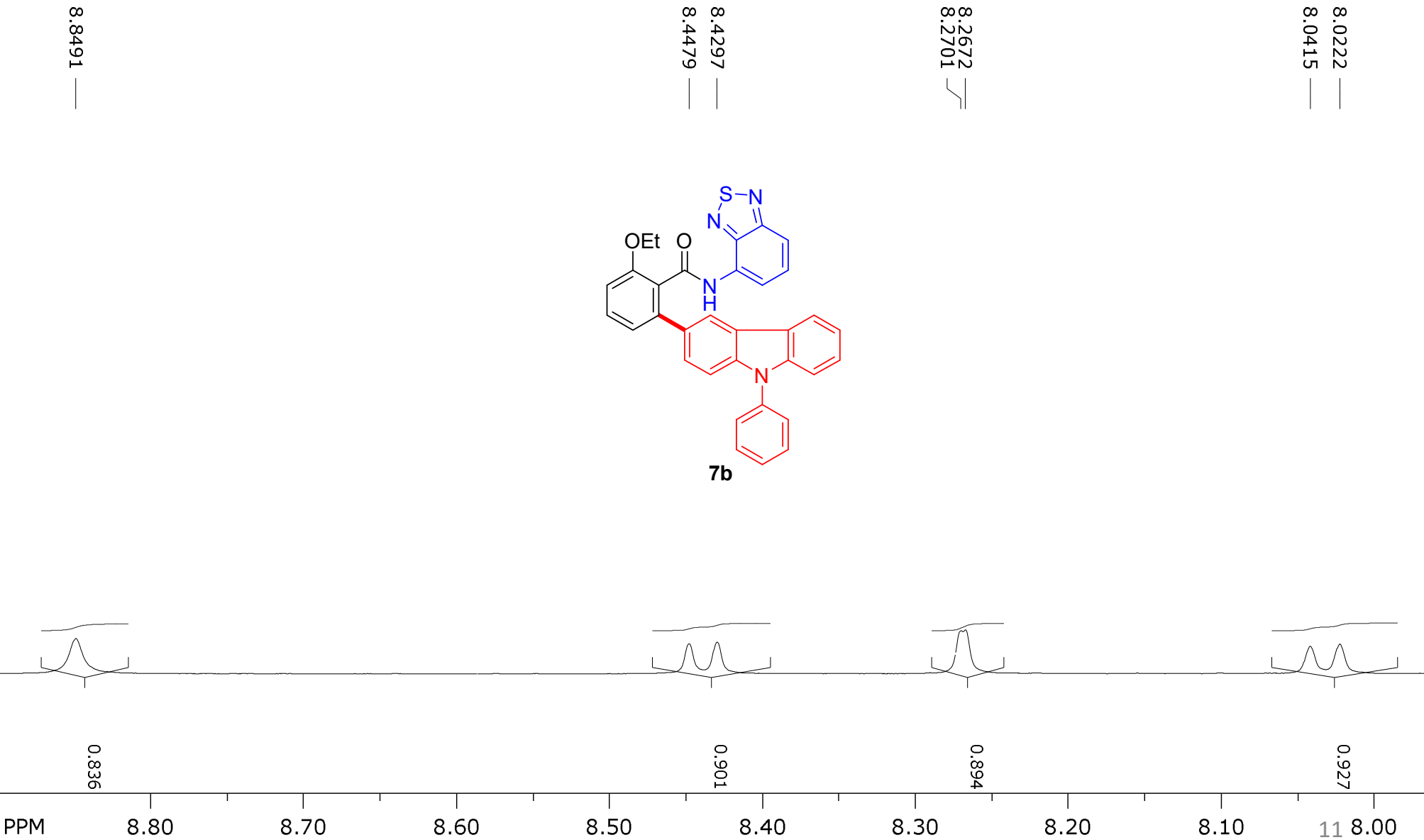
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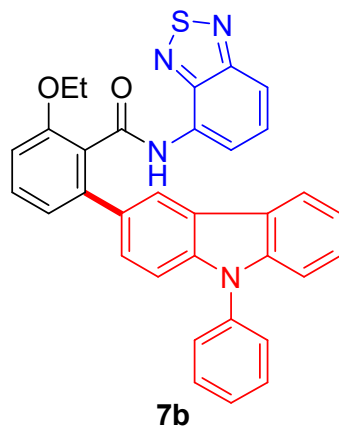


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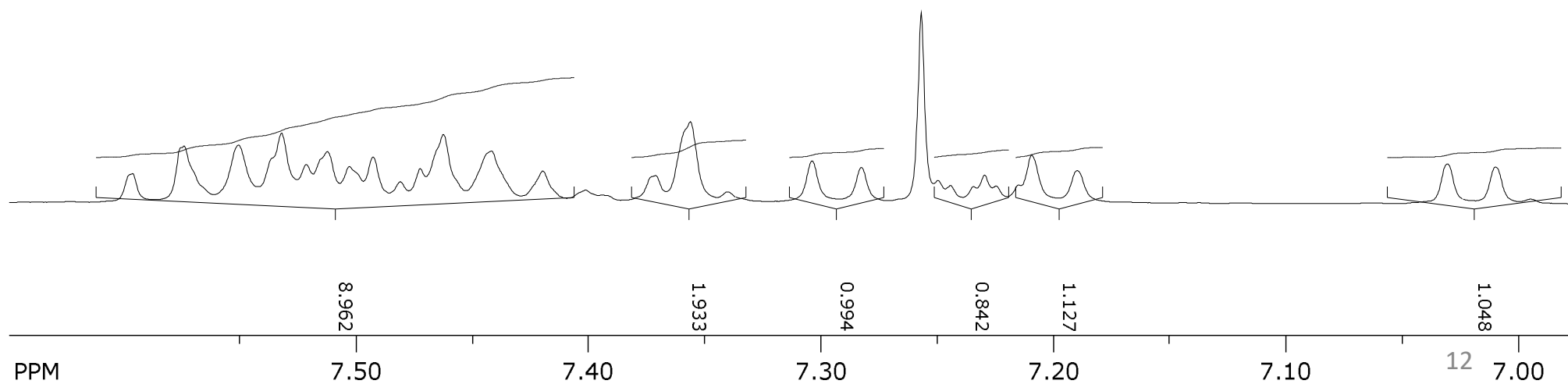


SpinWorks 4: RD-845-RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 42

7.5963	7.5740	7.5507	7.5321	7.5124	7.5030	7.4928	7.4810	7.4725	7.4625	7.4419	7.4197	7.3711	7.3562	7.3038	7.2826	7.2568	7.2496	7.2296	7.2093	7.1897	7.0304	7.0097
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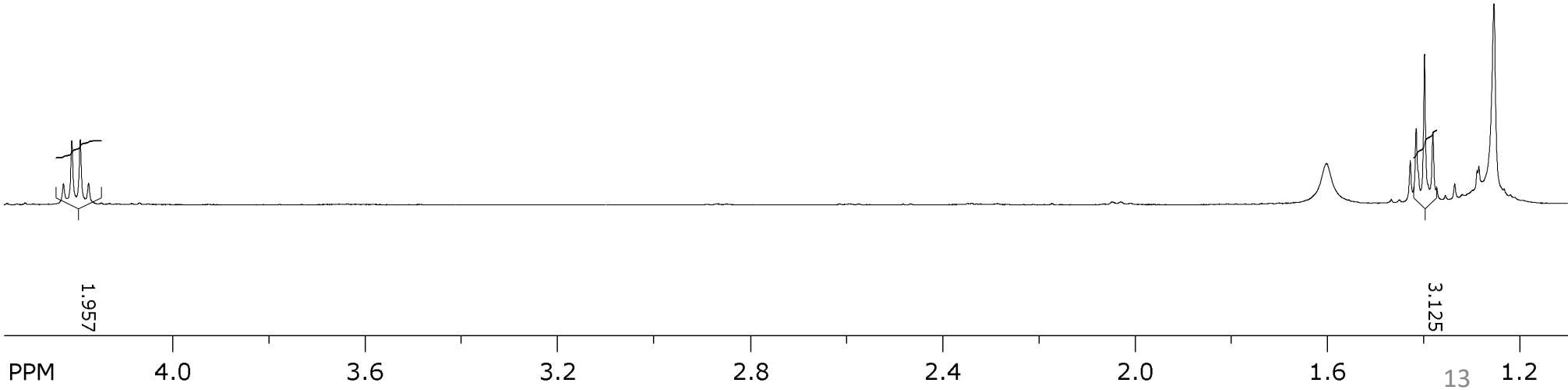
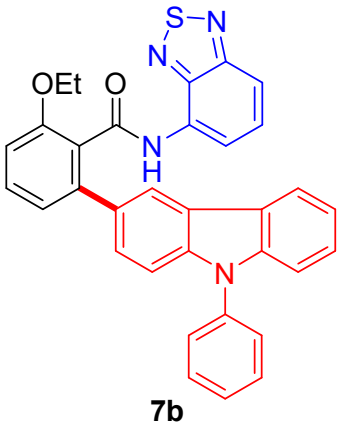
7b



SpinWorks 4: RD-845-RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 42

4.1755
4.1929
4.2104
4.2278

1.3804
1.3979
1.4152

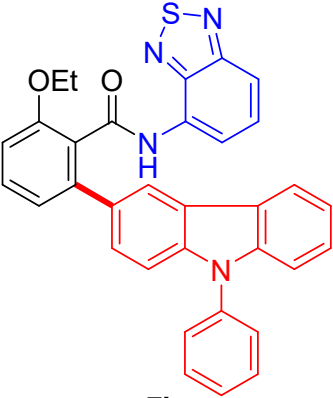


SpinWorks 4: RD-845-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 42

166.313
156.161
154.659
147.725
142.928
141.104
140.202
137.445
132.013
131.194
130.811
130.131
129.138
129.099
128.999
128.999
123.335
123.198
120.304
119.973
115.425
114.929
110.694
109.794
109.577

77.337
77.020
76.702
64.619

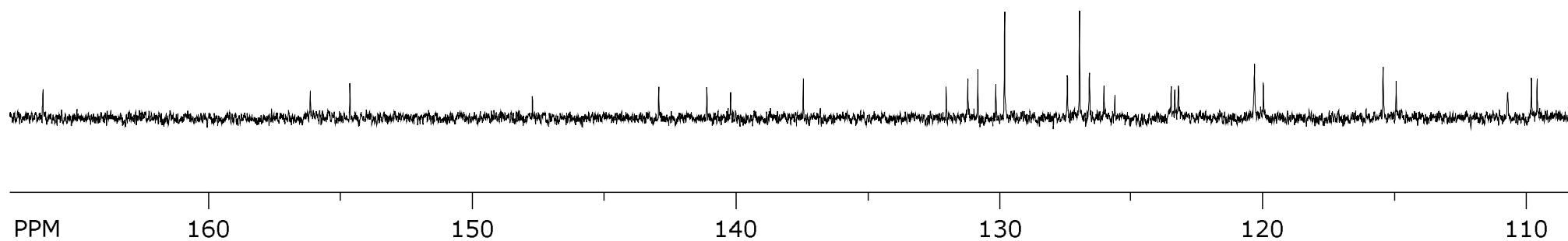
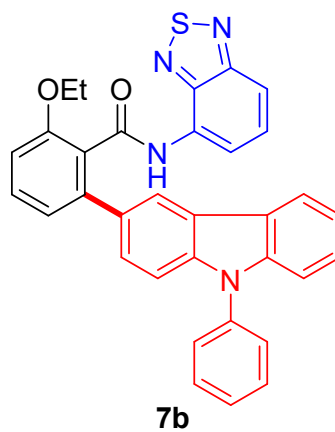
14.756



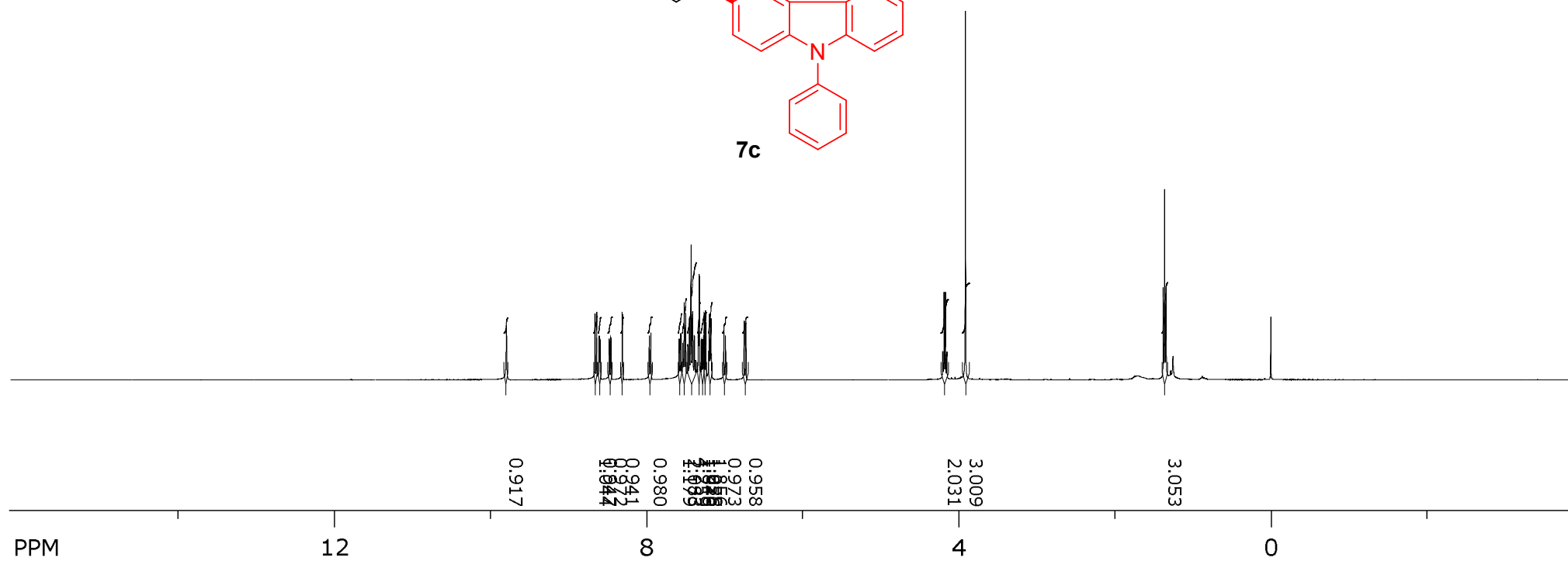
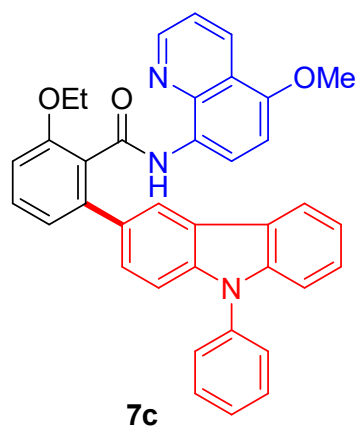
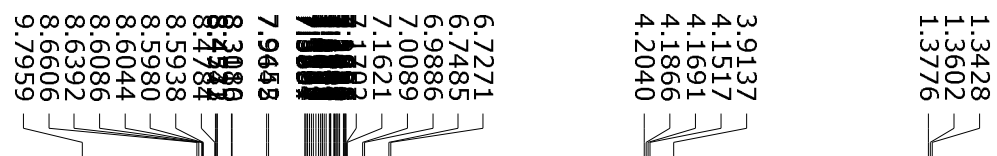
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SpinWorks 4: RD-845-RE
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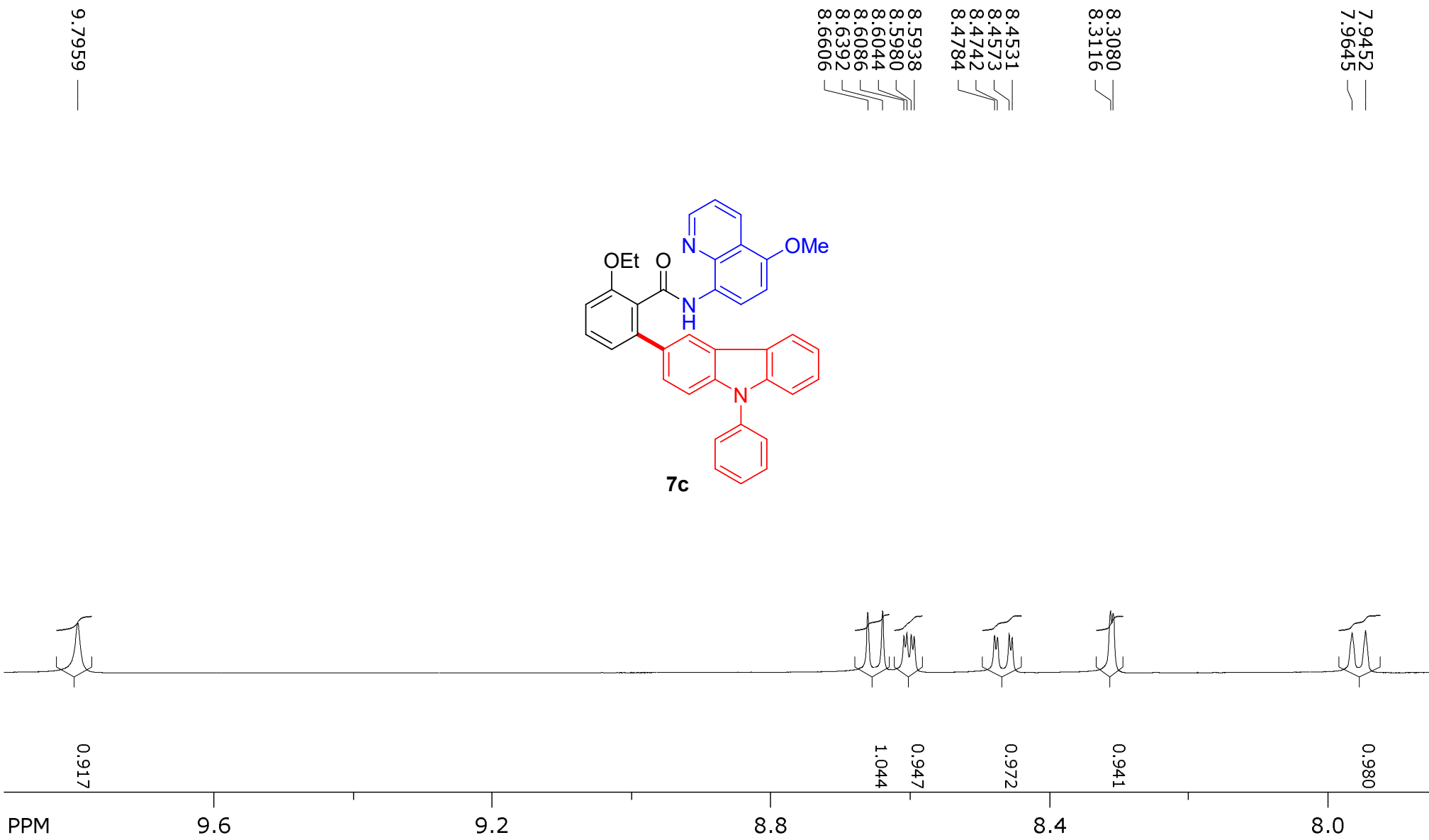
166.313 —
156.161 —
154.659 —
147.725 —
142.928 —
141.104 —
140.202 —
137.445 —
132.013 —
131.194 —
130.811 —
130.131 —
129.798 —
127.417 —
126.953 —
126.575 —
126.022 —
125.609 —
123.476 —
123.335 —
123.198 —
120.304 —
119.973 —
115.425 —
114.929 —
110.694 —
109.794 —
109.577 —



```
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41
```



SpinWorks 4: RD-823
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41



SpinWorks 4: RD-823

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

7.1621 —
7.1702 —
7.1757 —
7.1828 —
7.1893 —
7.1951 —
7.2026 —

7.2388 —
7.2471 —

7.2601 —
7.2661 —

7.2767 —
7.2872 —

7.2978 —

7.3243 —
7.3294 —
7.3360 —
7.3383 —

7.3720 —

7.3873 —

7.4093 —
7.4120 —

7.4303 —

7.4504 —

7.4705 —

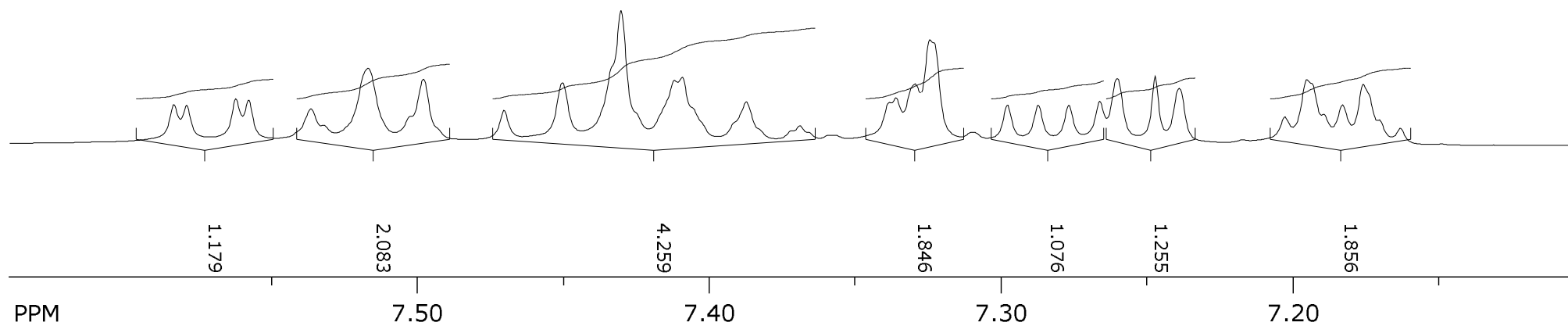
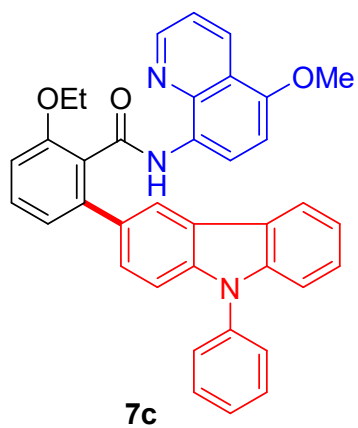
7.4981 —

7.5170 —

7.5367 —

7.5581 —
7.5624 —

7.5794 —
7.5837 —



SpinWorks 4: RD-823

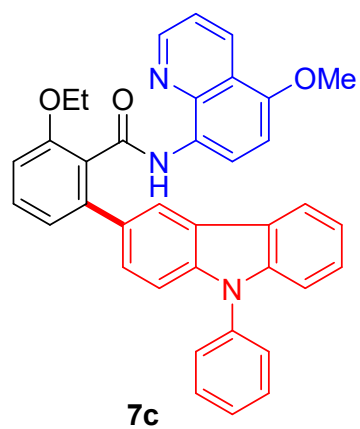
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7.0089

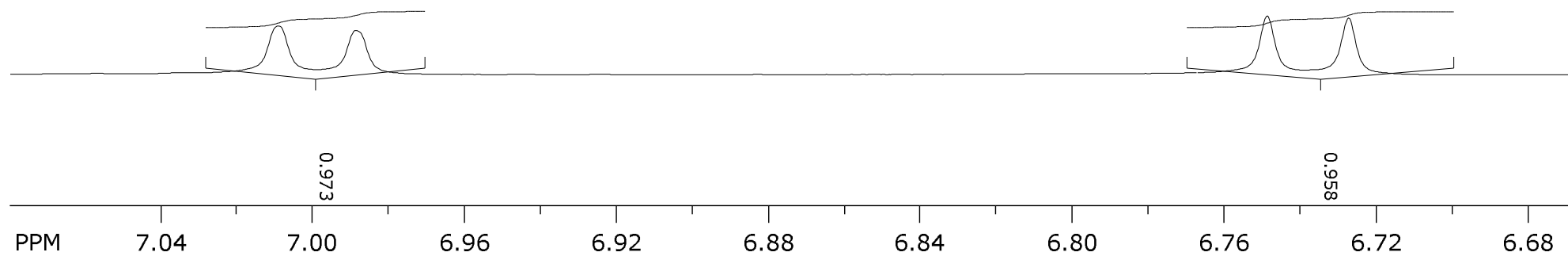
6.9886

6.7485

6.7271



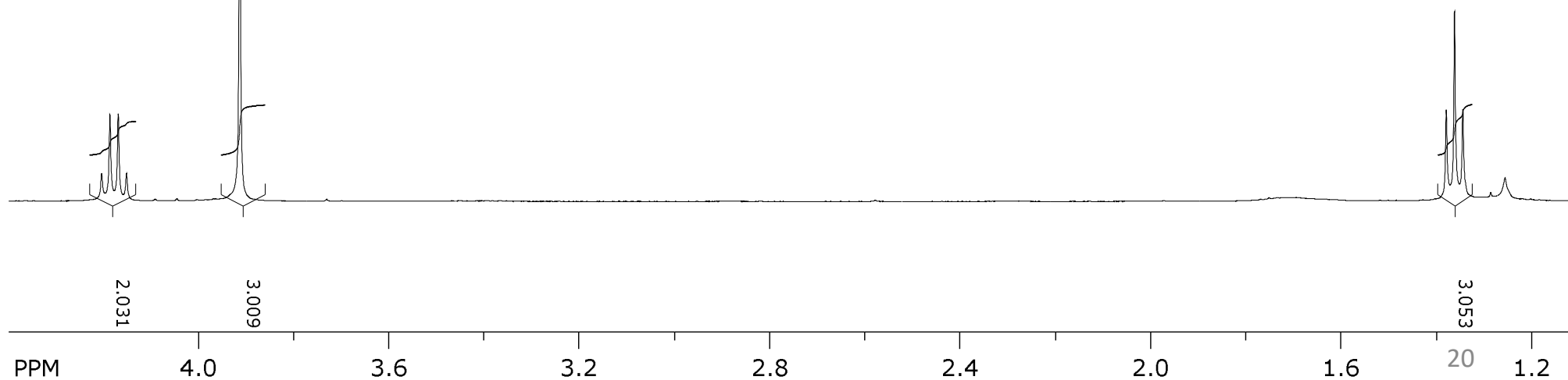
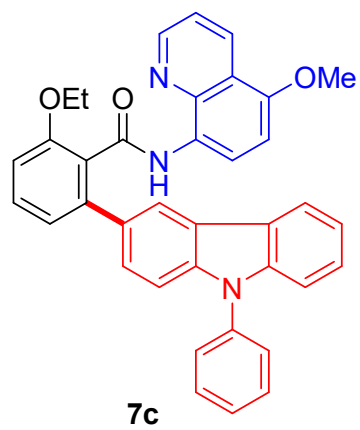
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SpinWorks 4: RD-823
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

4.1517
4.1691
4.1866
4.2040
3.9137

1.3428
1.3602
1.3776



SpinWorks 4: RD-823

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

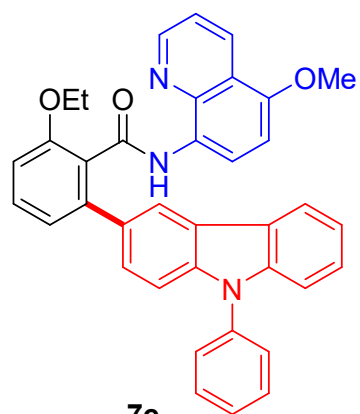
104.378
109.431
109.639
110.759
116.781
119.789
120.236
120.283
120.429
121.989
122.989
123.989
129.989
130.102
130.867
132.372
137.581
139.190
140.141
141.039
142.525
148.330
150.073
156.163
165.880

76.702
77.020
77.337

64.519

55.689

14.726



PPM

160

120

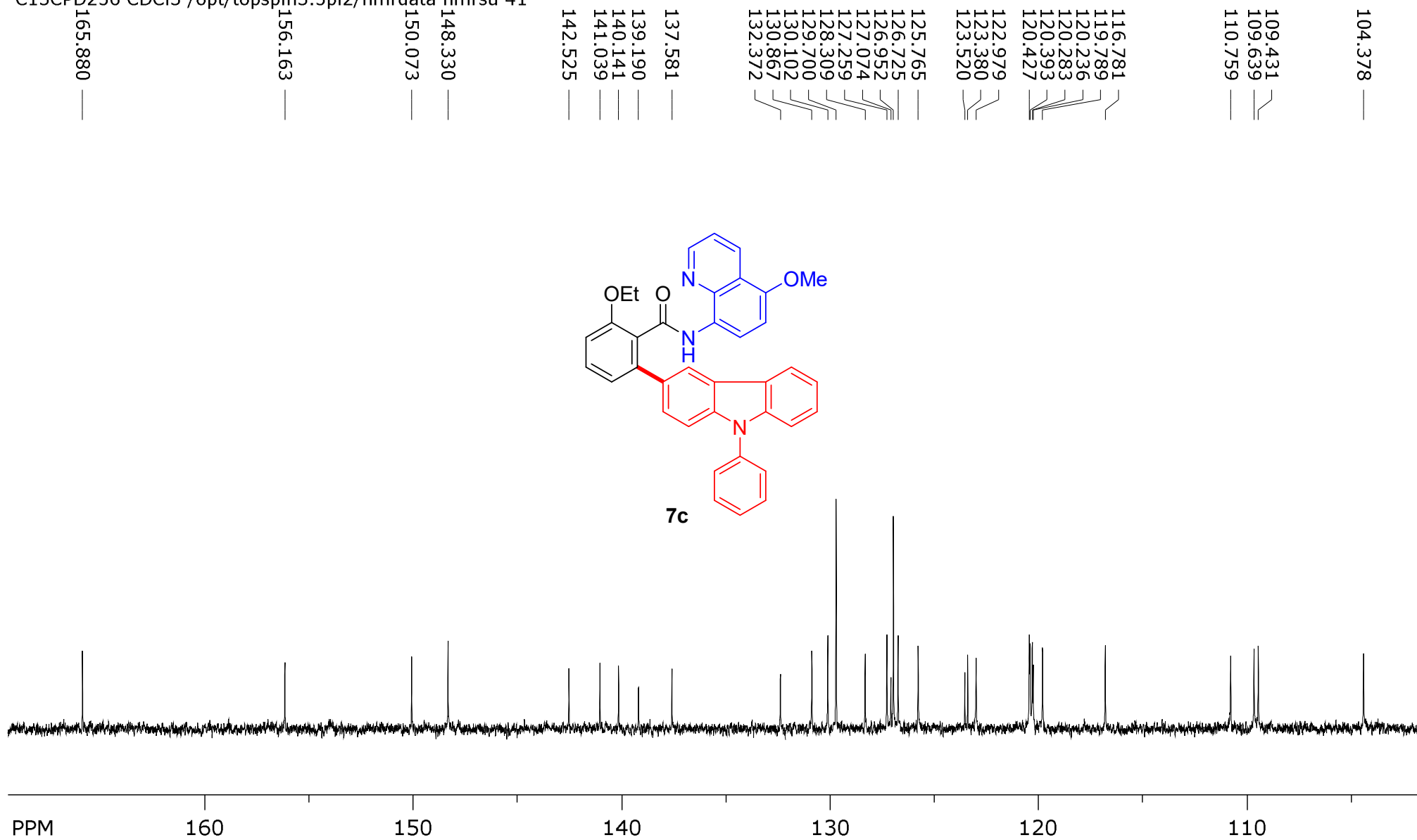
80

40

01

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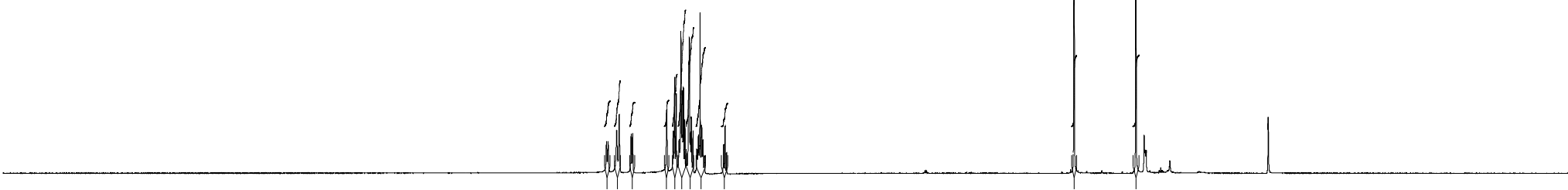
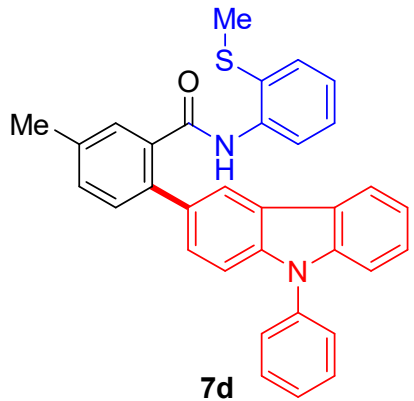
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SpinWorks 4: RD-817
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

6.9125
6.9152
6.9314
6.9339
6.9503
6.9529
7.1955
7.1955
7.1955
7.1955
7.1955
7.1955
7.5743
7.5743
7.5938
7.6763
8.1116
8.1309
8.2830
8.3153
8.4247
8.4451

1.6871
2.4757



PPM 12 8 4 0 23

SpinWorks 4: RD-817

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8.4451

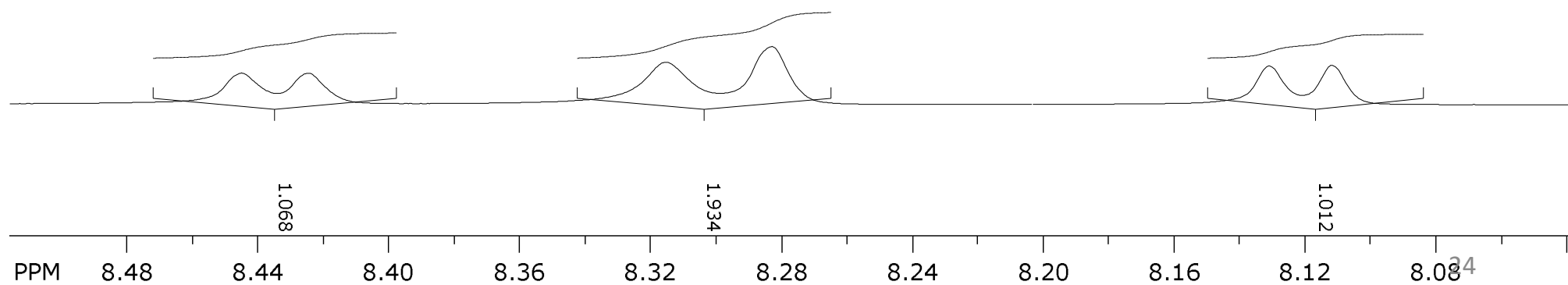
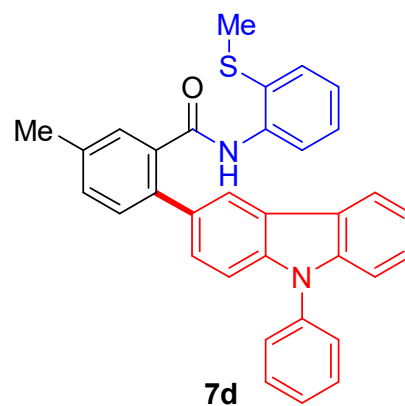
8.4247

8.3153

8.2830

8.1309

8.1116

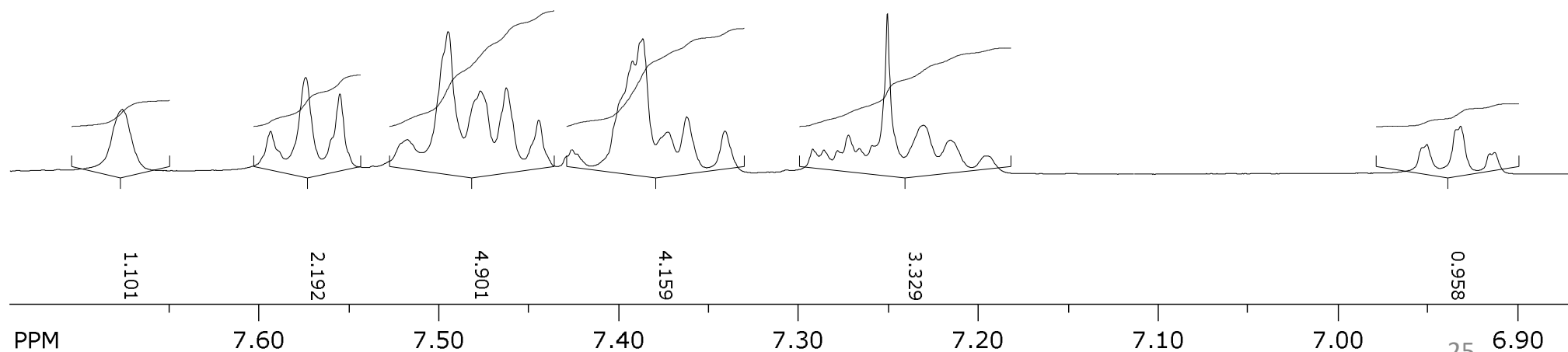
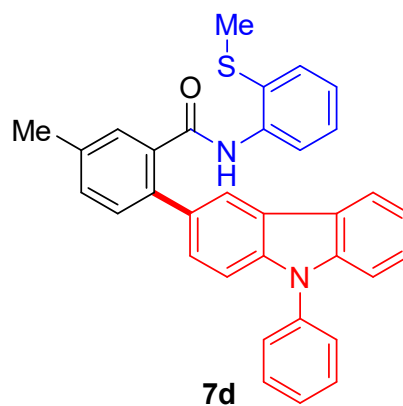


SpinWorks 4: RD-817

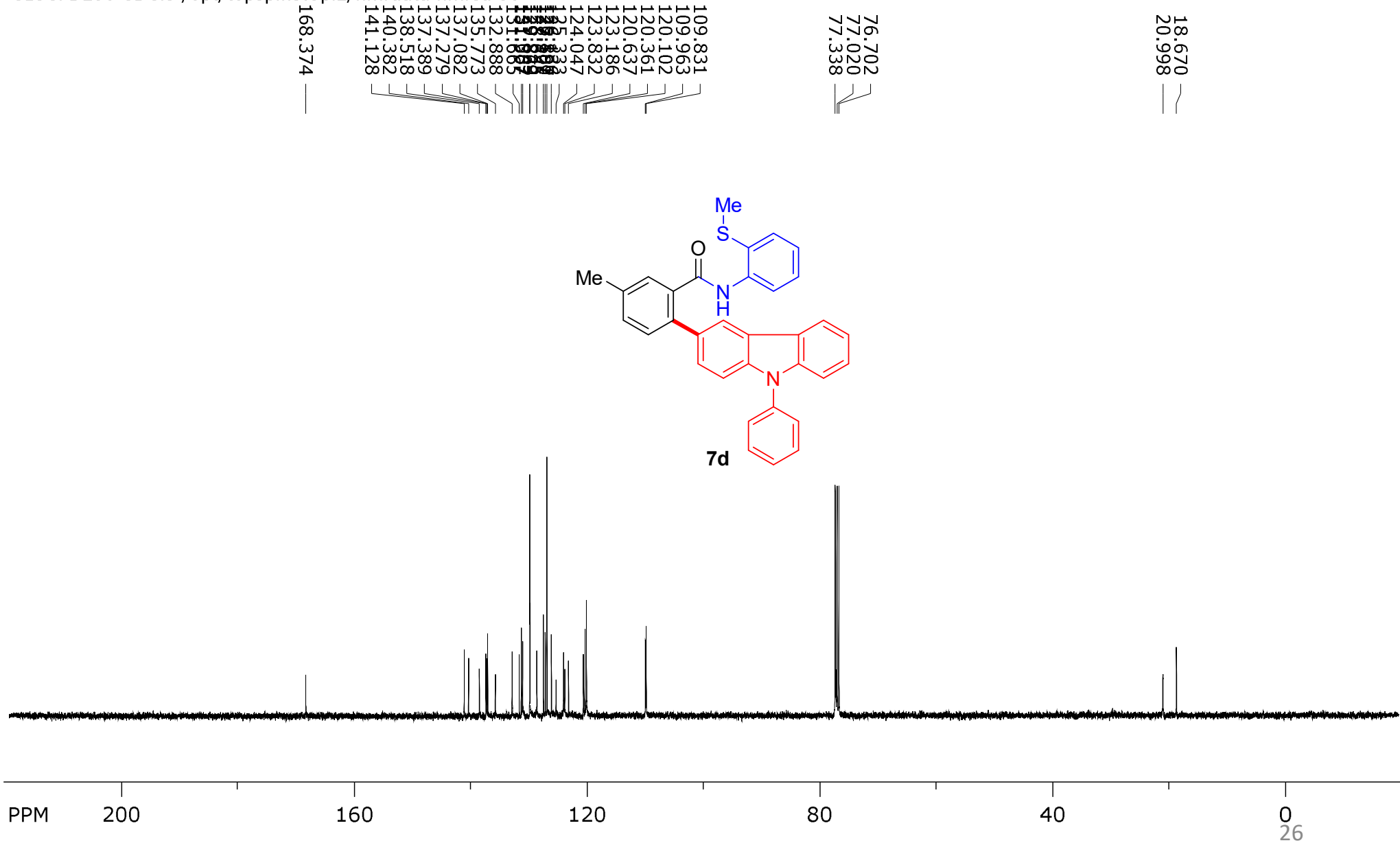
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6.9125
6.9152
6.9314
6.9339
6.9503
6.9529

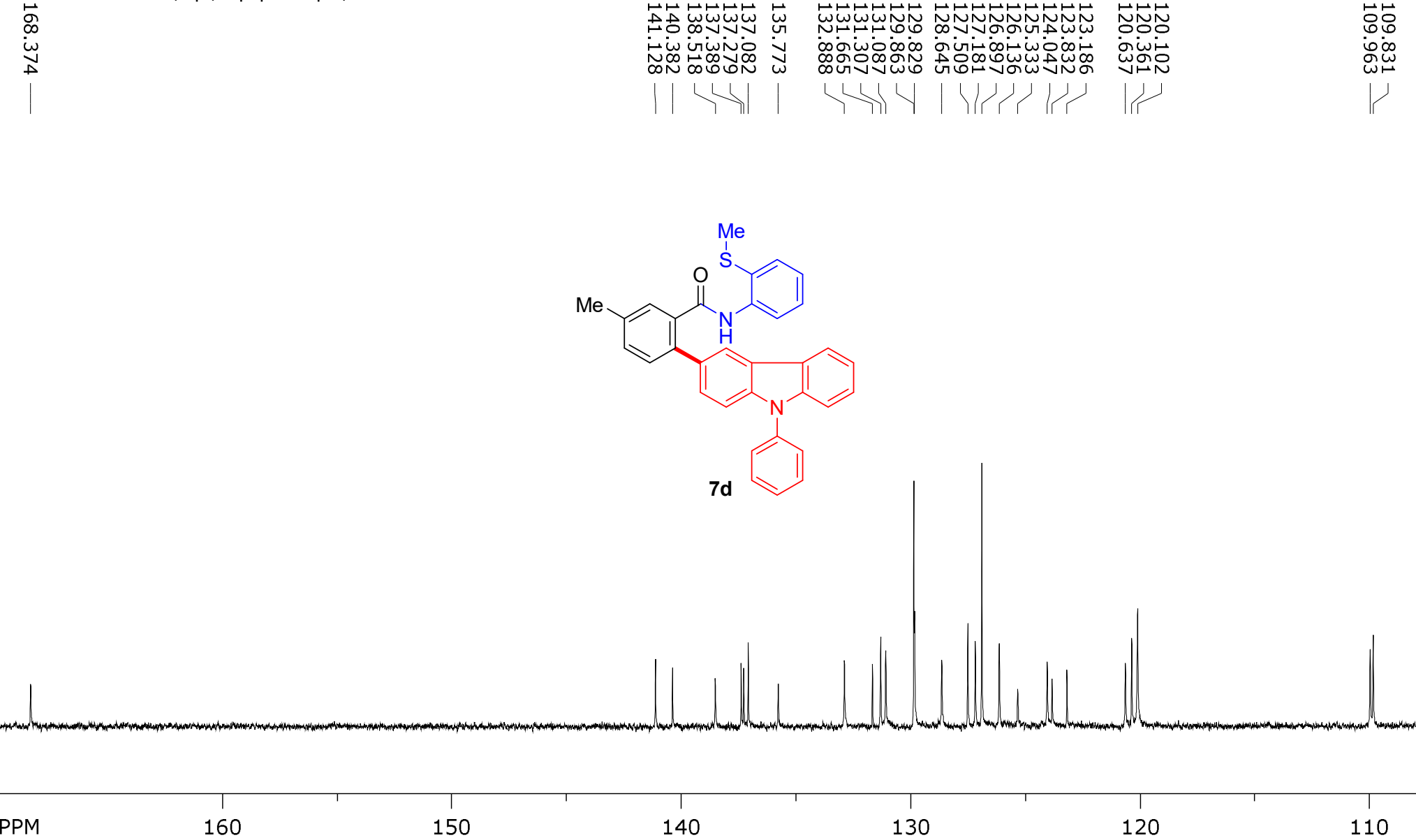
7.1955
7.2155
7.2304
7.2505
7.2589
7.2661
7.2722
7.2782
7.2858
7.2921
7.3409
7.3621
7.3724
7.3866
7.3924
7.4235
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7.4949
7.5178
7.5552
7.5743
7.5938
7.6763



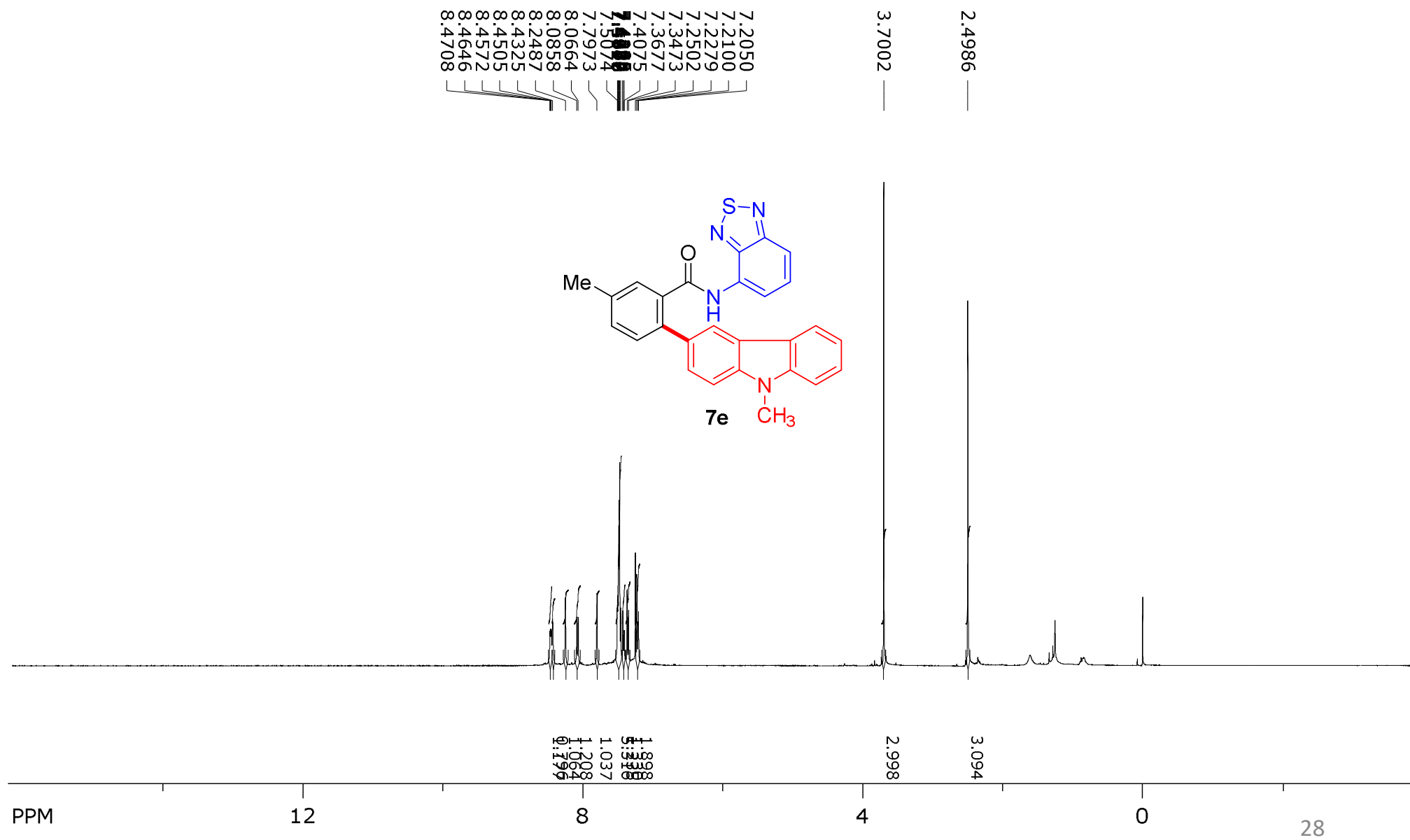
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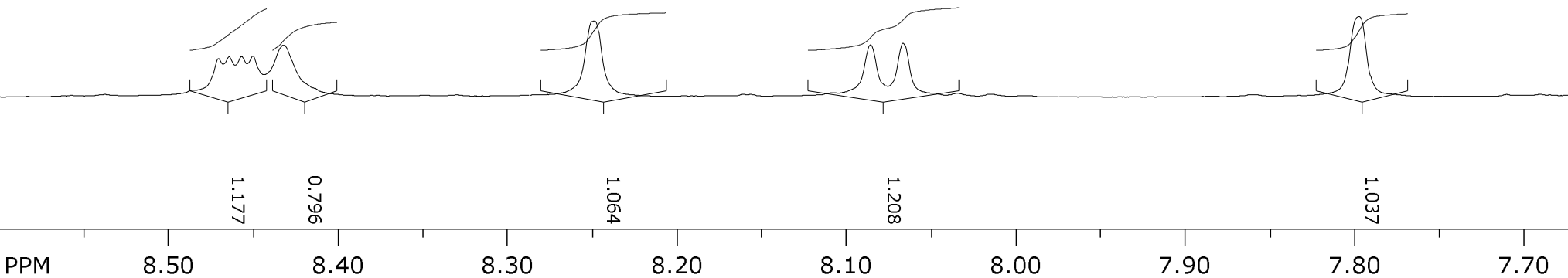
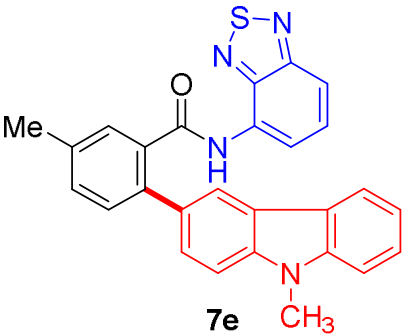
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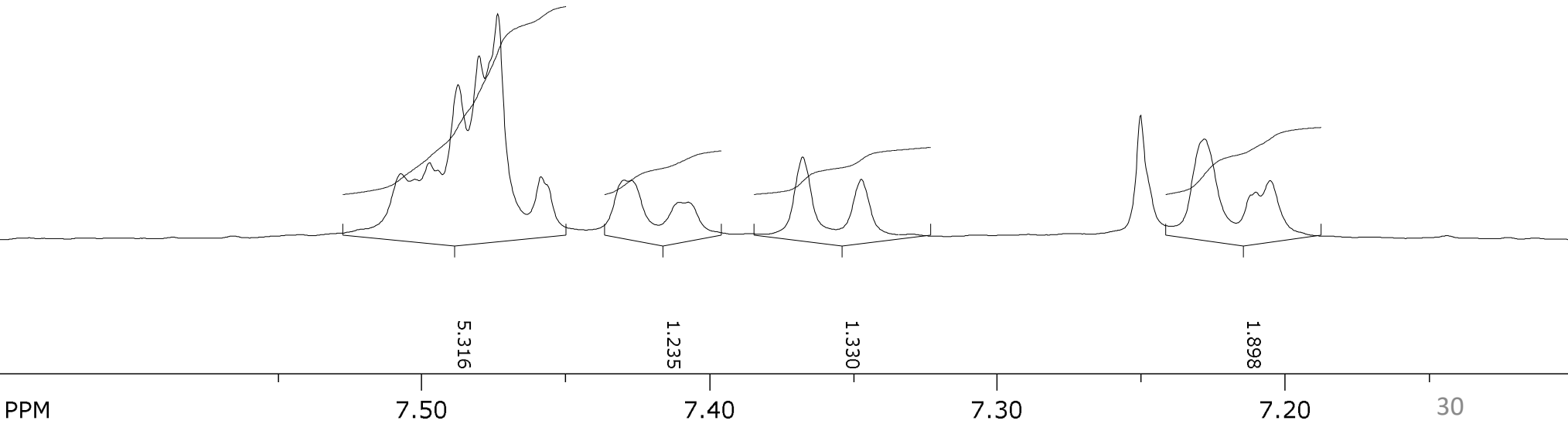
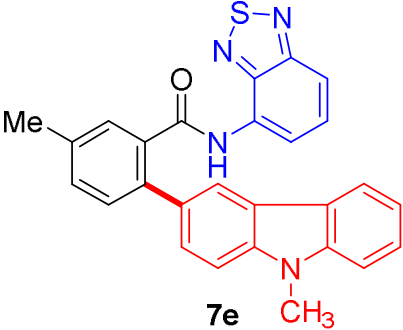


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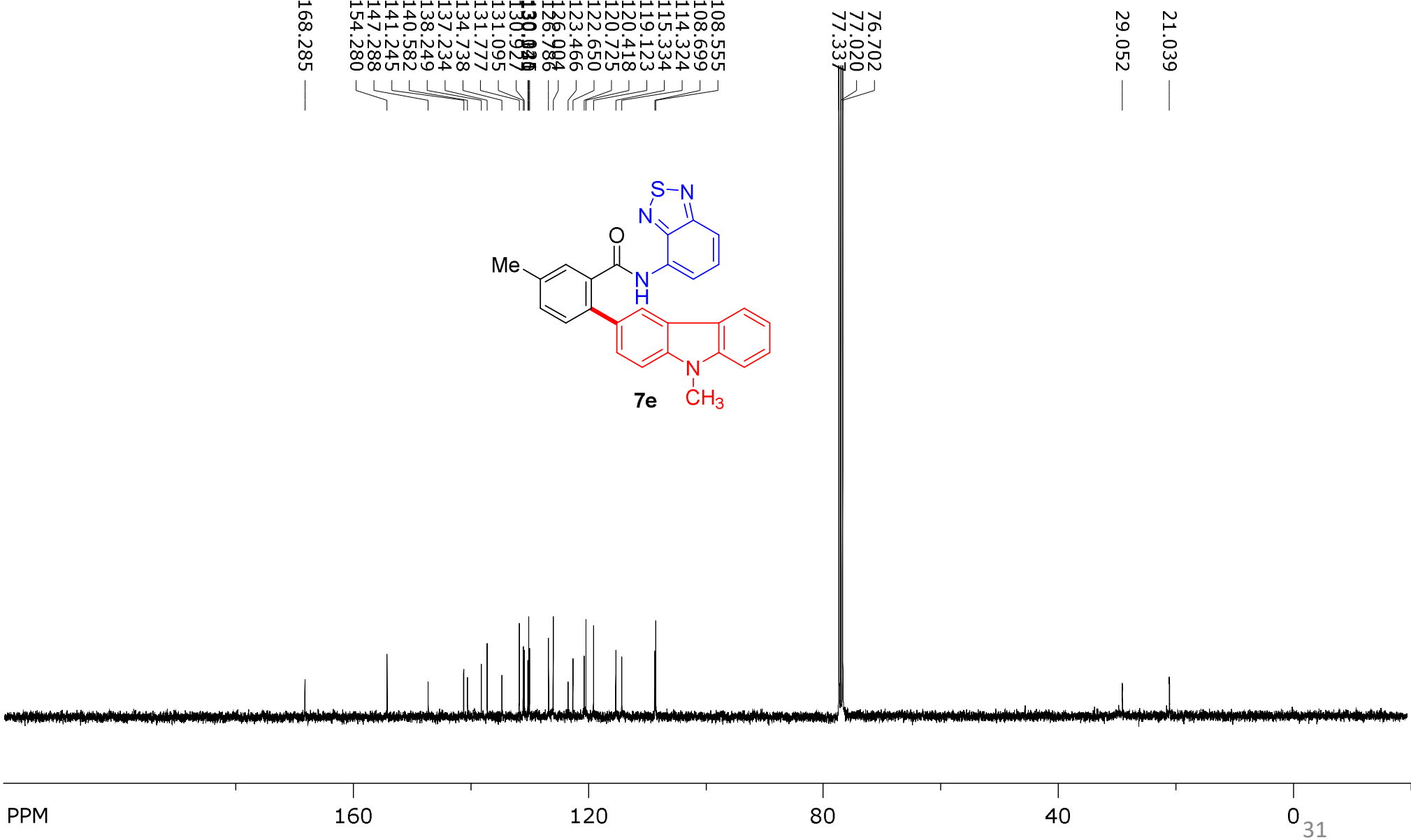
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7.4587	7.4075	7.3473	7.2050
7.4738	7.4105	7.3677	7.2100
7.4802	7.4273		
7.4876	7.4298		
7.4947			
7.4975			
7.5026			
7.5074			

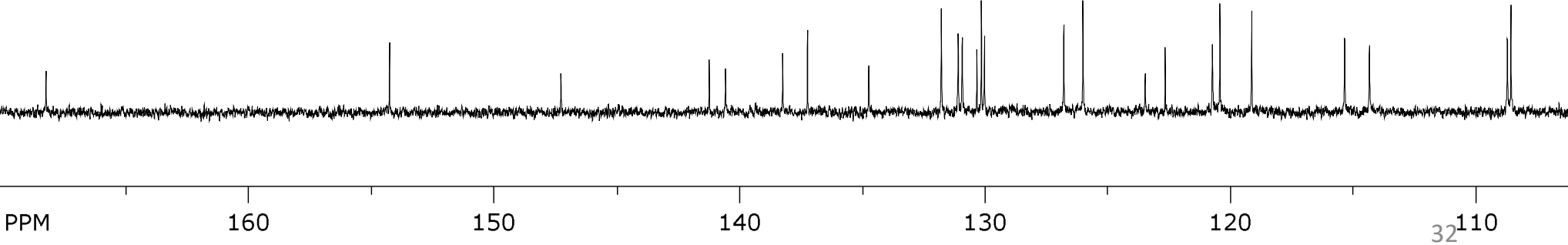
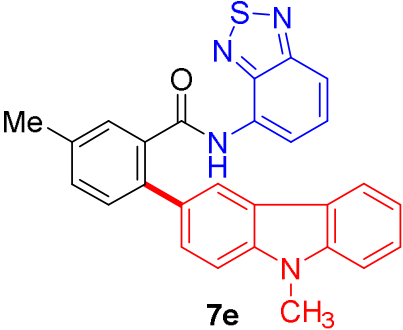
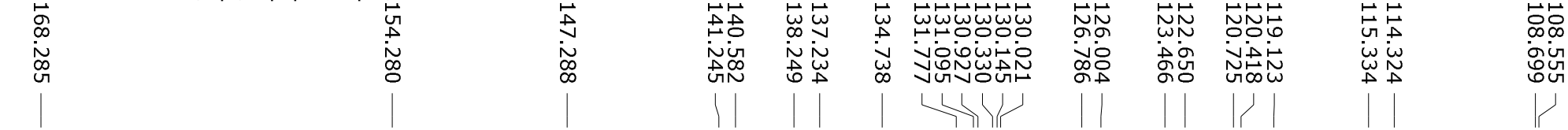


SpinWorks 4: RD-764

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



SpinWorks 4: RD-764
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



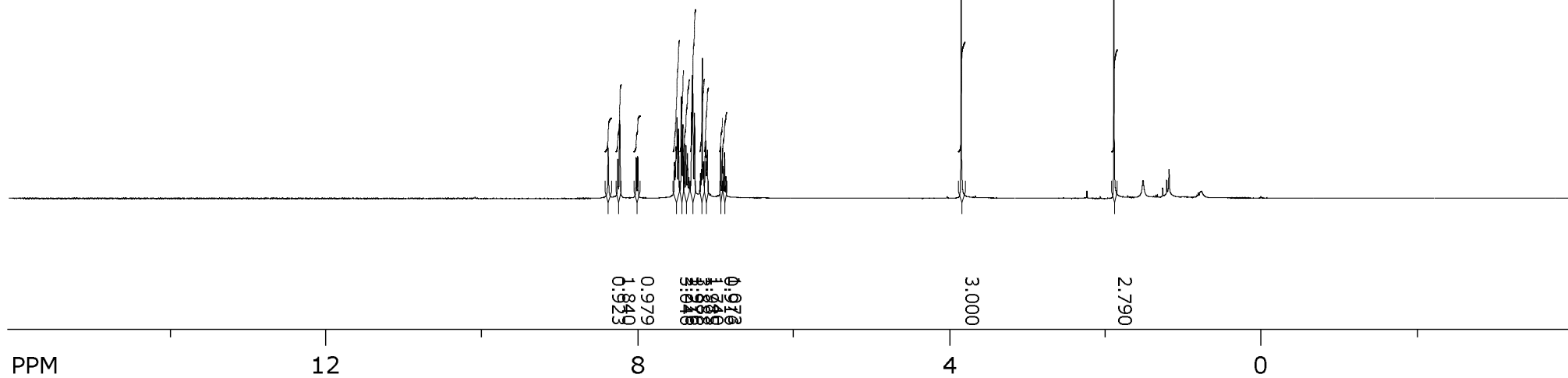
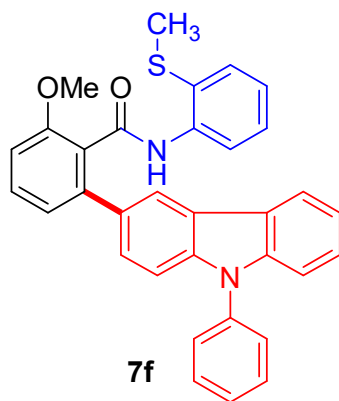
SpinWorks 4: RD-858

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

6.8657
6.8683
6.8847
6.8869
6.9036
6.9065
6.9135
7.1904
7.1904
7.1904
7.5137
7.5255
7.5291
7.9988
8.0182
8.2303
8.2544
8.3787

3.8479

1.8862



SpinWorks 4: RD-858
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

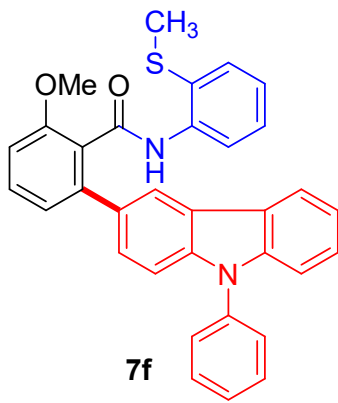
8.3787

8.2544

8.2303

8.0182

7.9988

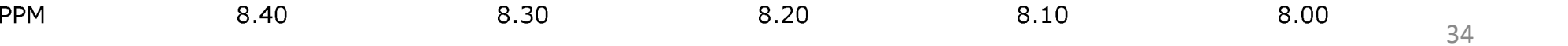


7f

0.923

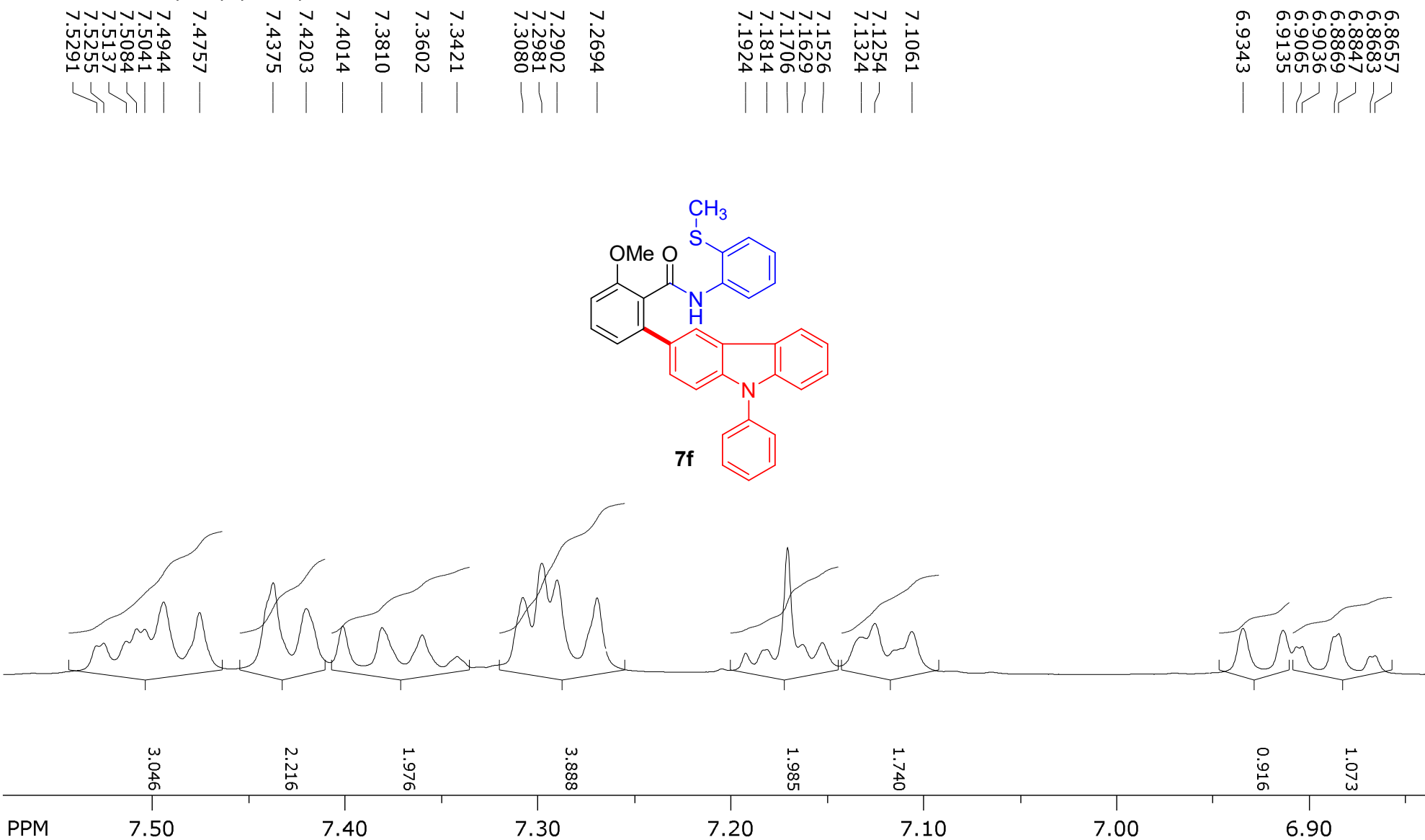
1.840

0.979



SpinWorks 4: RD-858

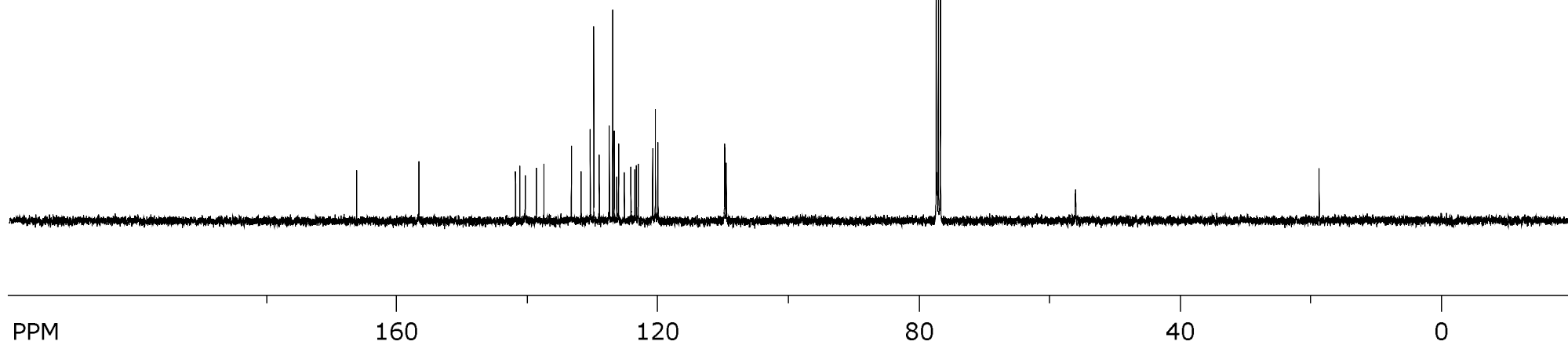
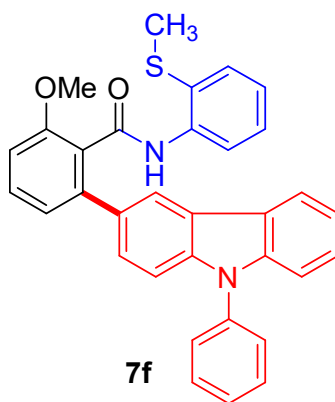
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40



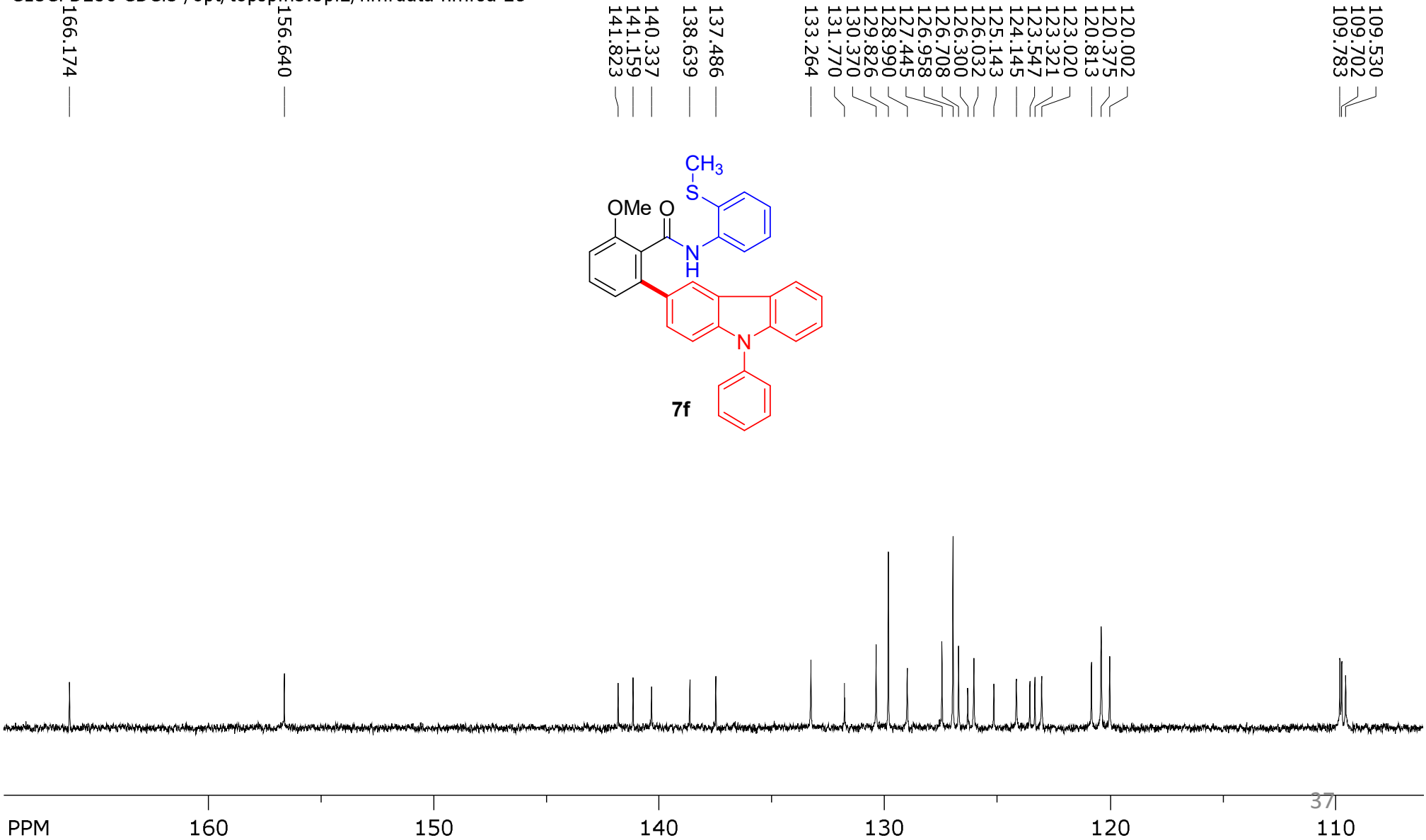
SpinWorks 4: RD-858

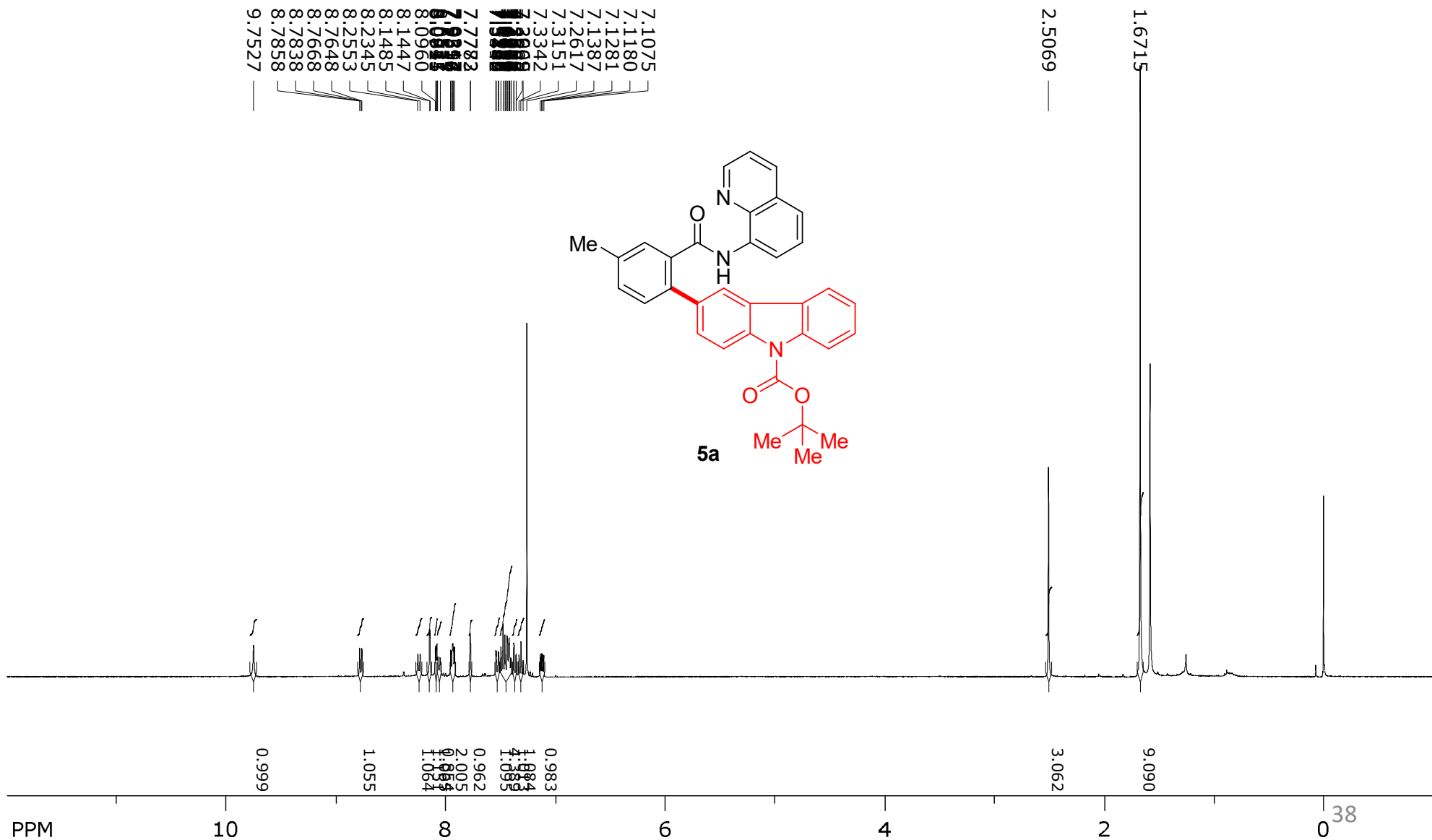
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28

166.174
156.640
141.823
141.159
140.337
138.639
137.486
133.264
131.770
130.370
129.826
128.990
128.199
128.199
128.199
123.547
123.321
123.020
120.813
120.375
120.002
109.783
109.702
109.530
76.703
77.020
77.338
55.979
18.672



SpinWorks 4: RD-858
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28





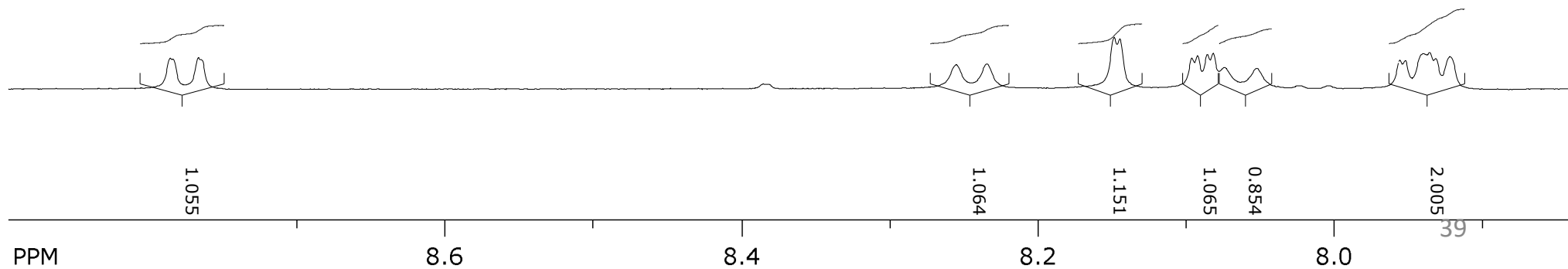
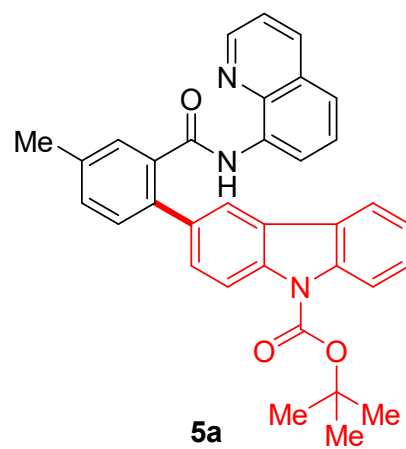
SpinWorks 4: rd-152

8.7648
8.7668
8.7838
8.7858

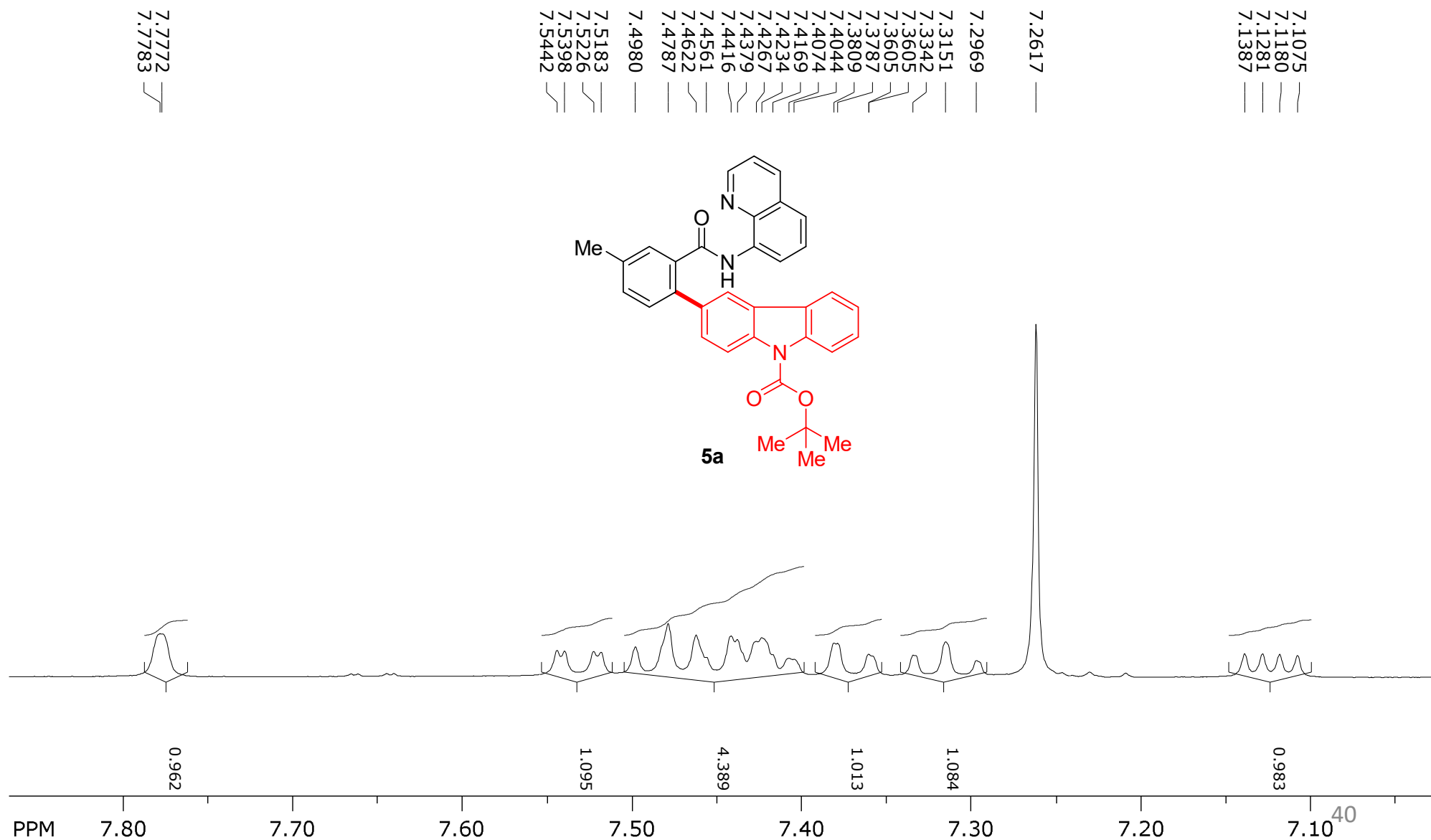
8.2345
8.2553

8.0522
8.0741
8.0815
8.0855
8.0921
8.0960
8.1447
8.1485

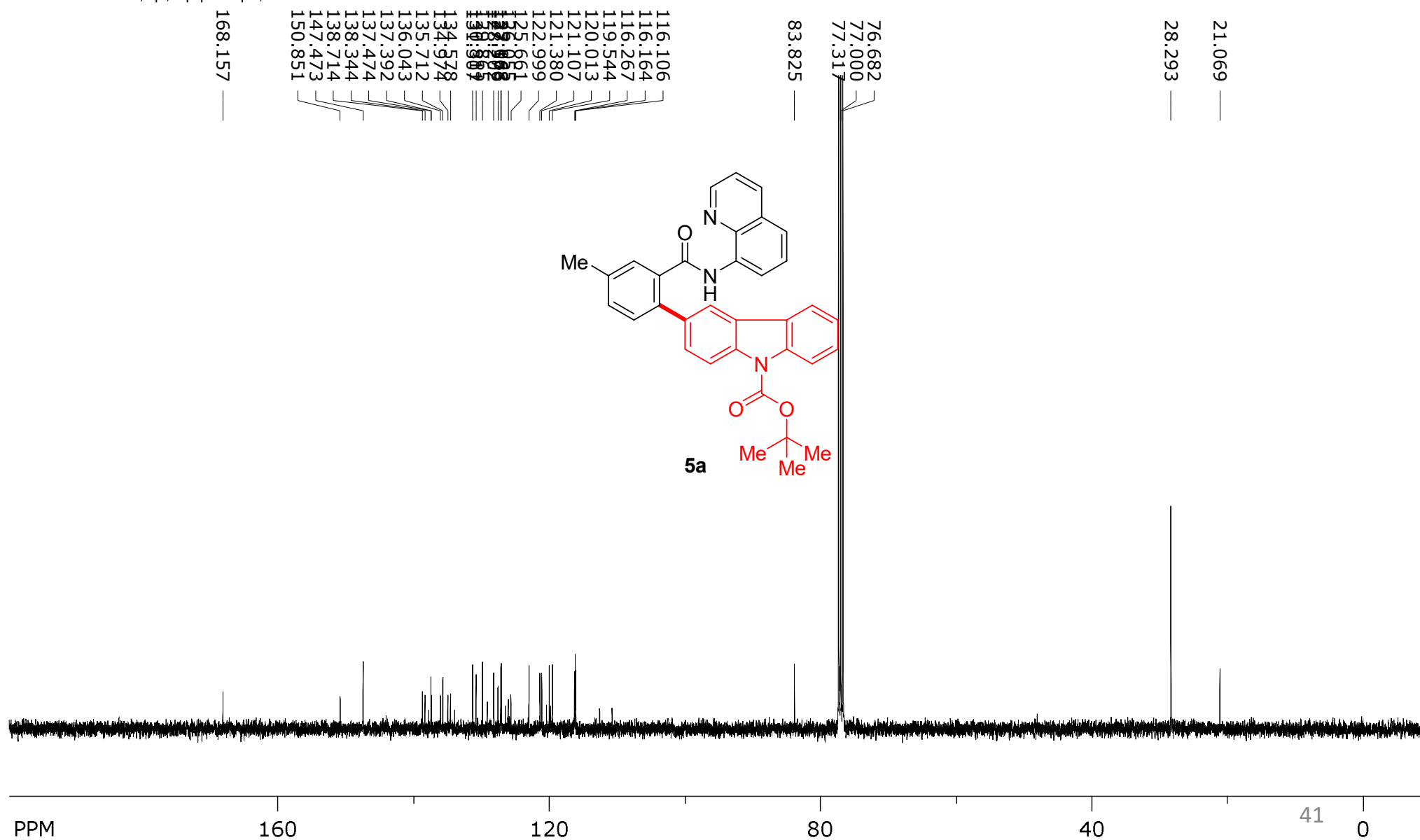
7.9217
7.9313
7.9354
7.9397
7.9518
7.9556



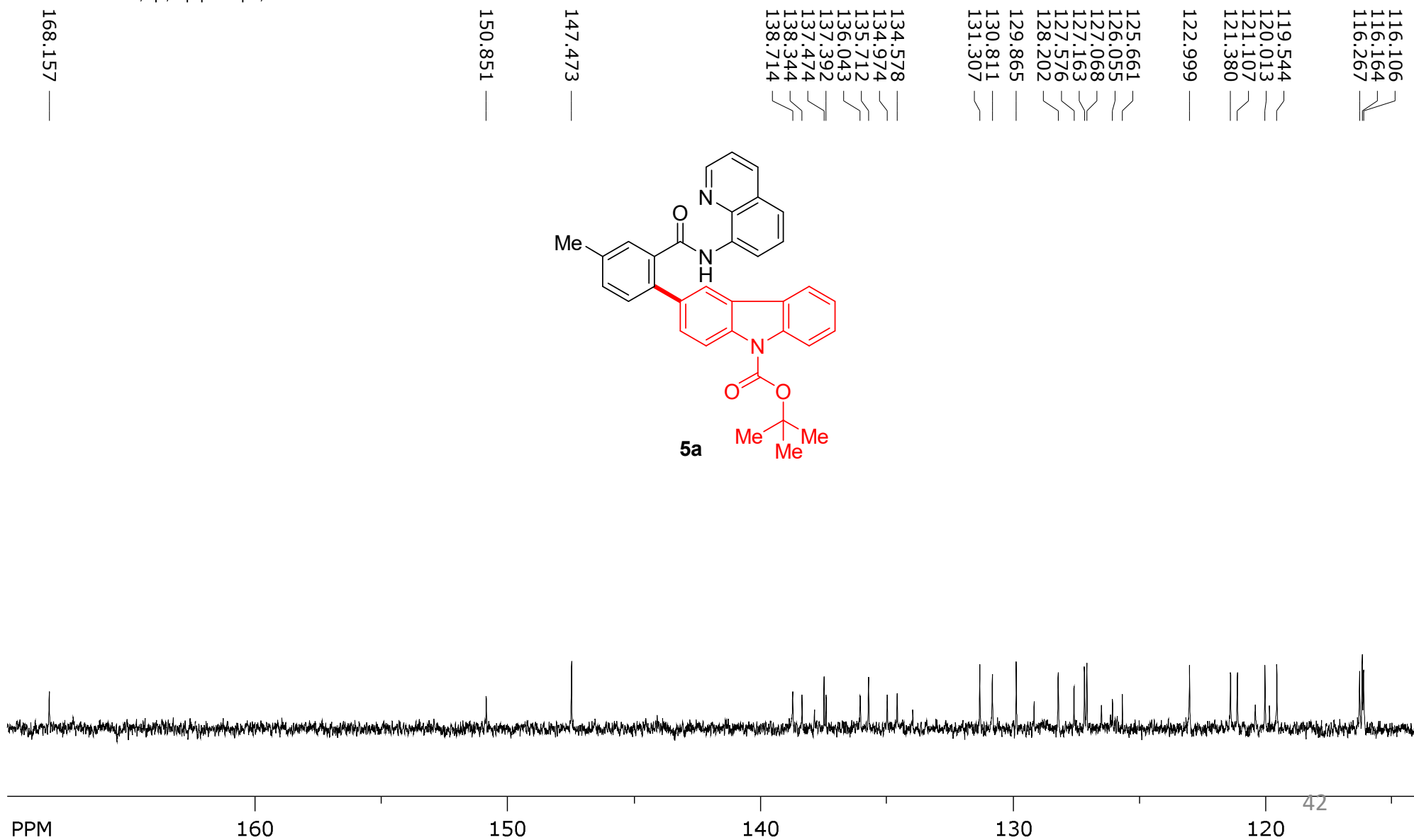
SpinWorks 4: rd-152



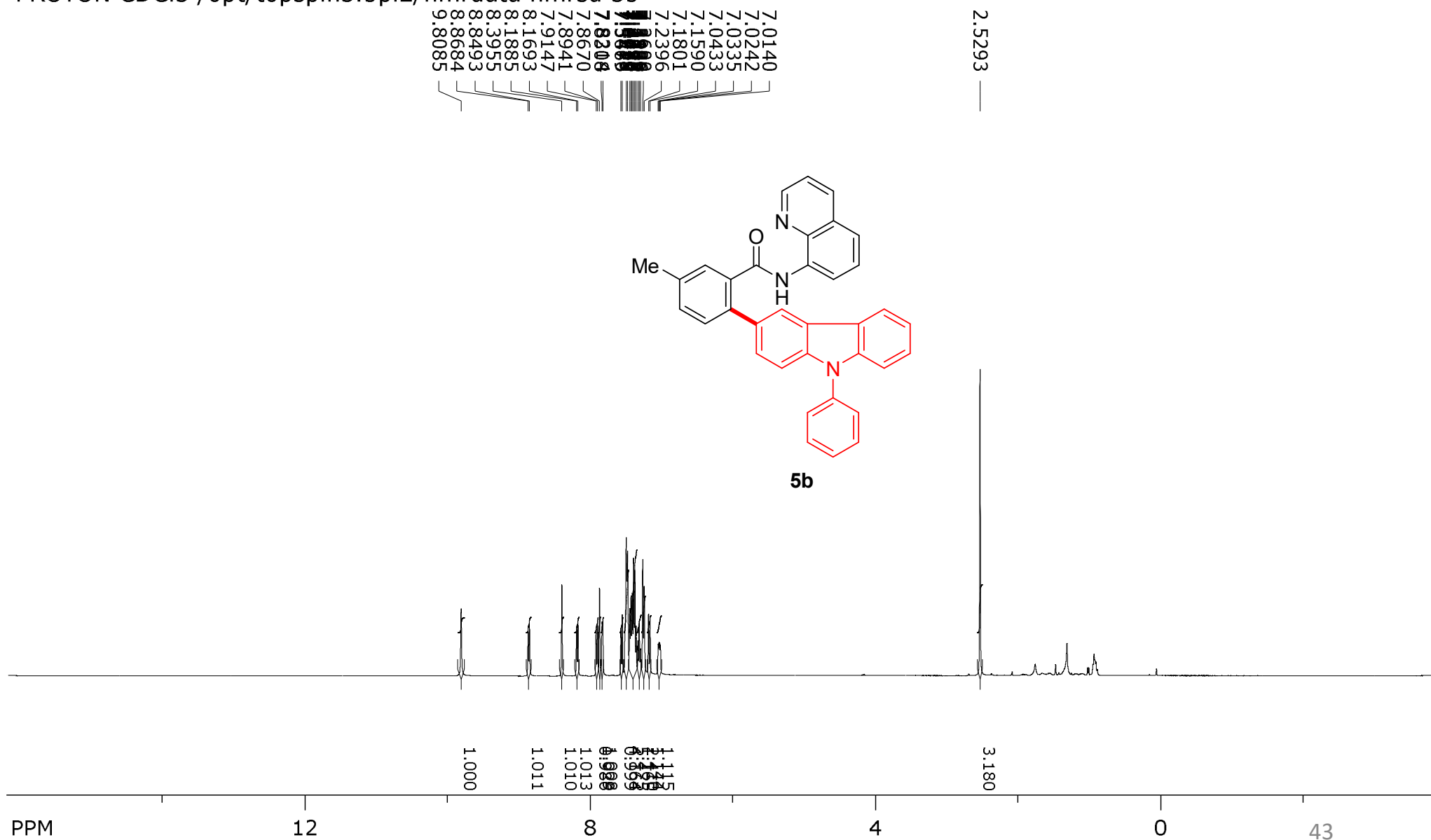
SpinWorks 4: RD 152
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



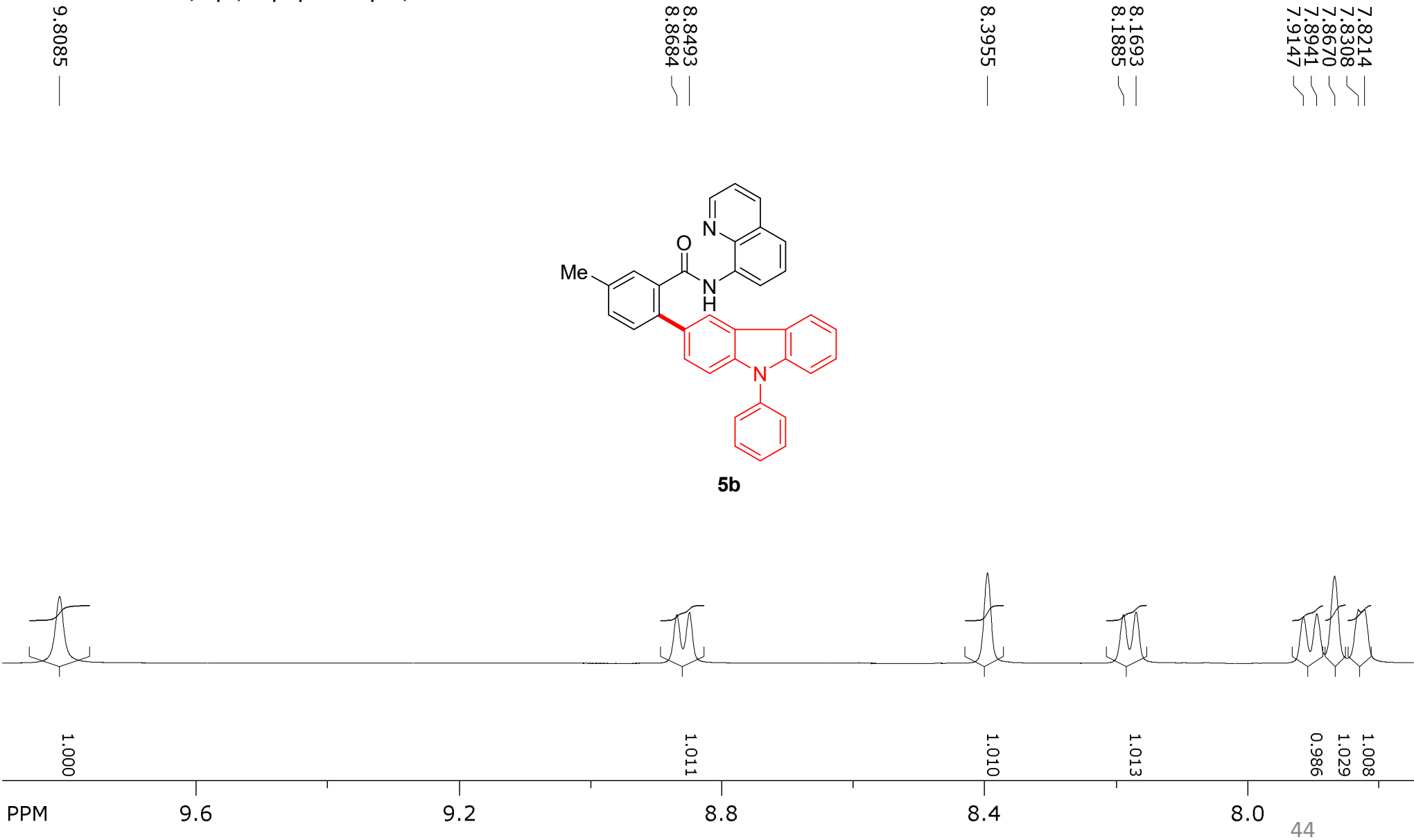
SpinWorks 4: RD 152
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 35

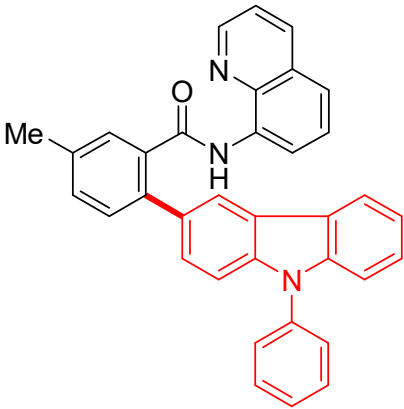


SpinWorks 4: rd-144
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 35

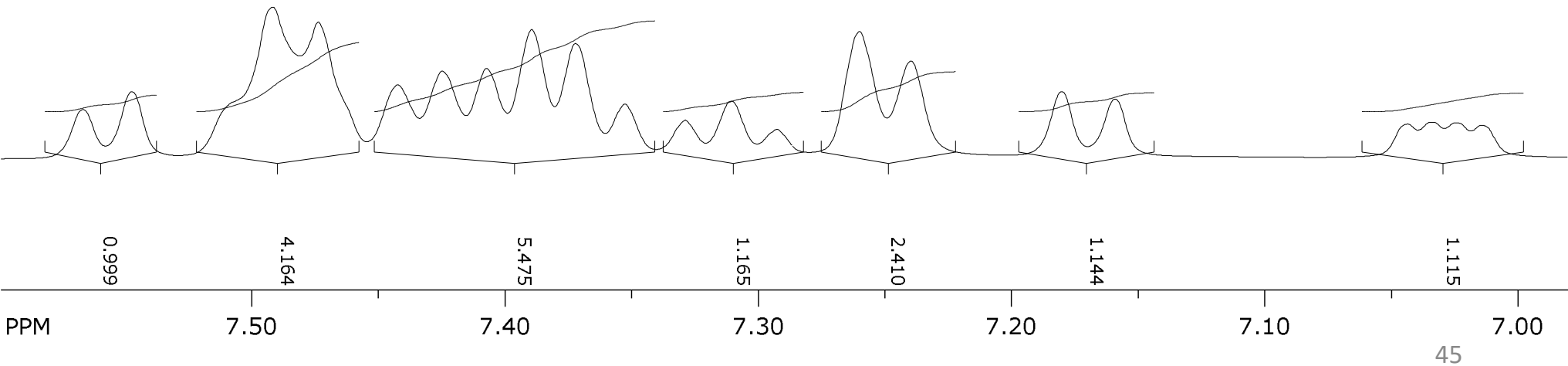


SpinWorks 4: rd-144
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 35

7.5669 —
7.5476 —
7.4919 —
7.4739 —
7.4425 —
7.4250 —
7.4075 —
7.3896 —
7.3723 —
7.3527 —
7.3289 —
7.3106 —
7.2926 —
7.2600 —
7.2396 —
7.1801 —
7.1590 —
7.0433 —
7.0335 —
7.0242 —
7.0140 —

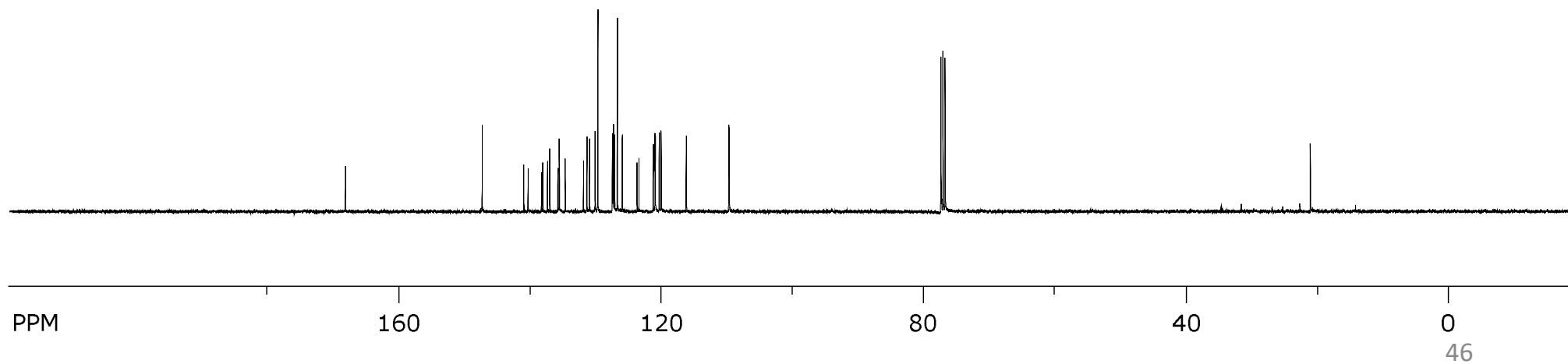
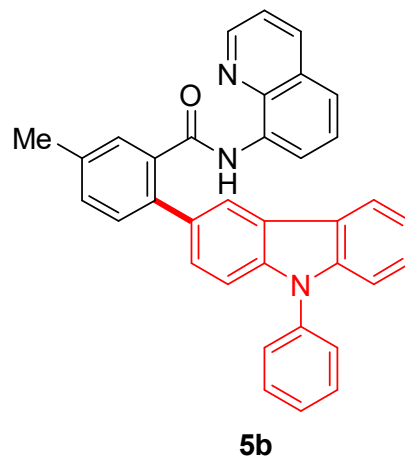


5b



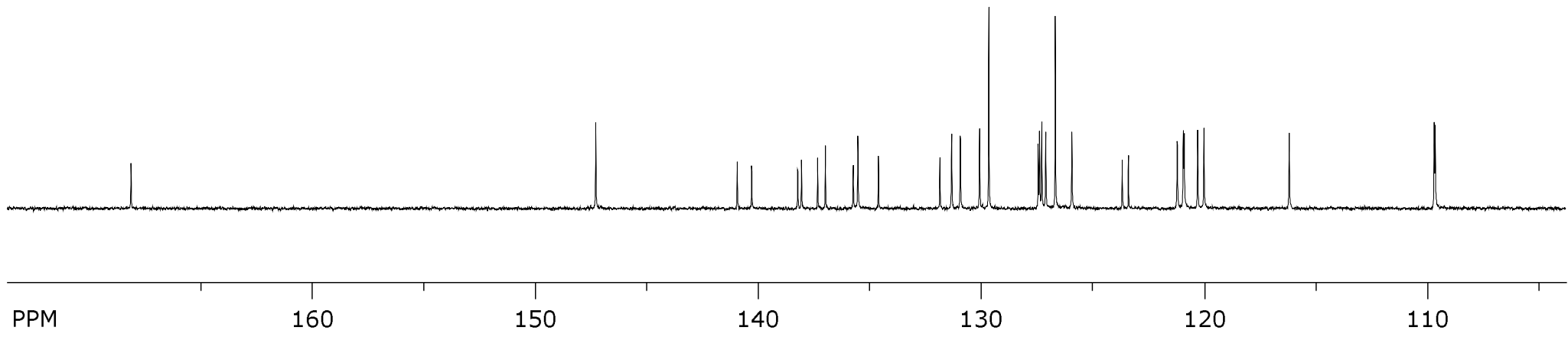
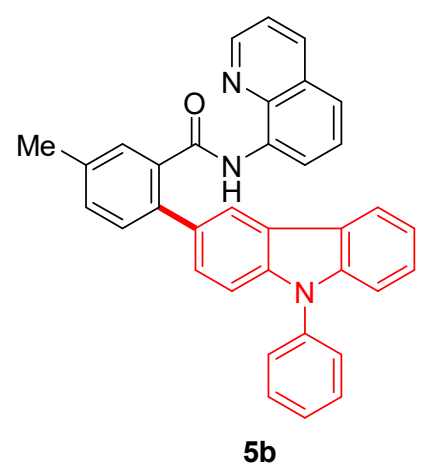
C13CPD256 CDCl3 /opt/topspin3.5p2/nmrdata/nmr su 4

21.003	76.702	109.632
	77.020	109.677
	77.338	116.181
		120.003
		120.291
		120.893
		120.934
		121.202
		123.098
		130.000
		130.000
		130.000
		133.514
		135.741
		136.990
		137.338
		138.066
		138.234
		140.298
		140.943
		147.290
		156.148

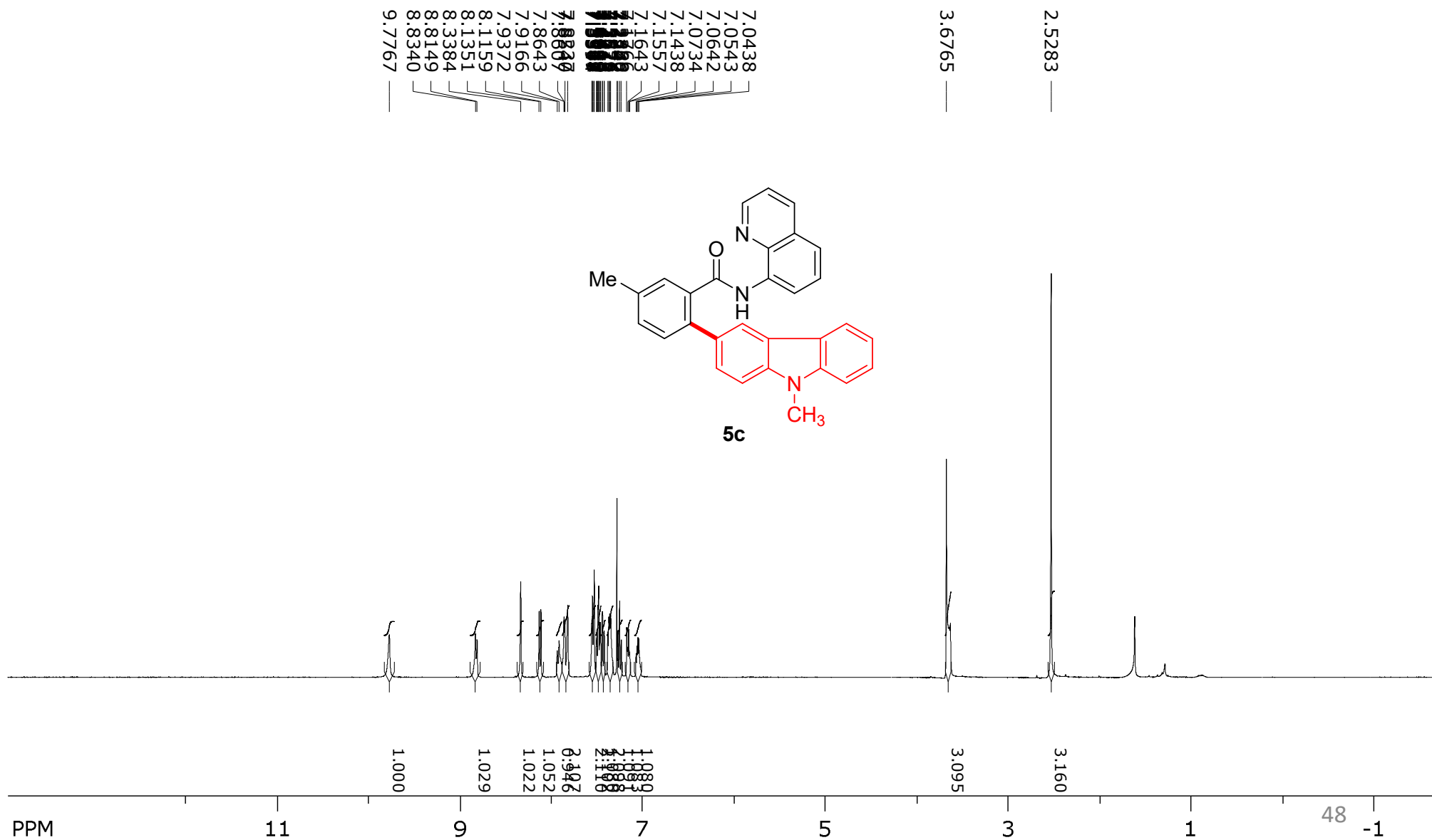


SpinWorks 4: RD 144
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

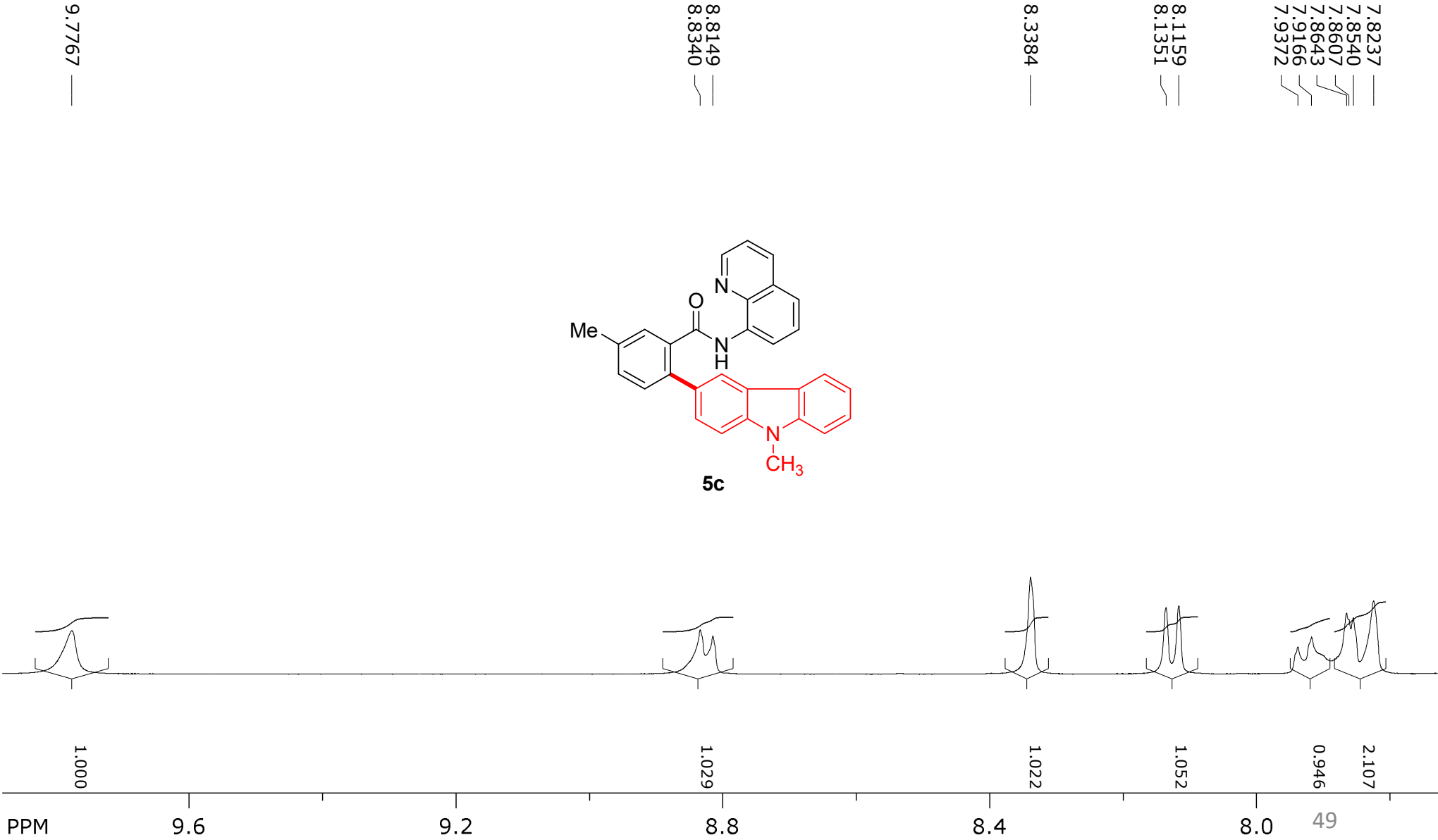
168.148	147.290	140.943	138.234	137.338	136.990	135.741	135.532	134.614	131.856	131.322	130.935	130.076	129.656	127.445	127.385	127.283	127.106	126.679	125.932	123.676	123.392	121.202	120.934	120.893	120.291	120.003	116.181	109.677	109.632
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SpinWorks 4: RD-1211
 PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28

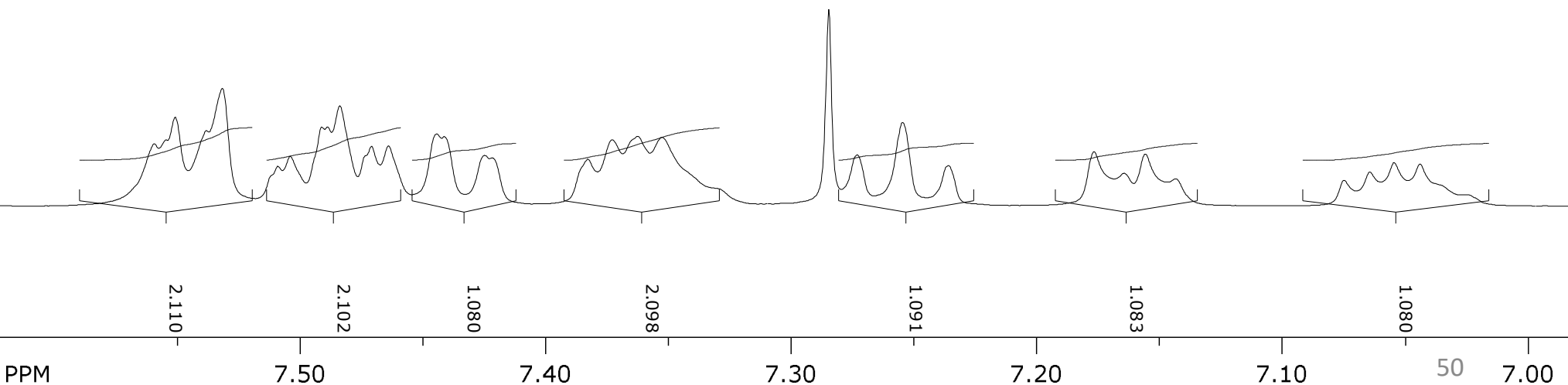
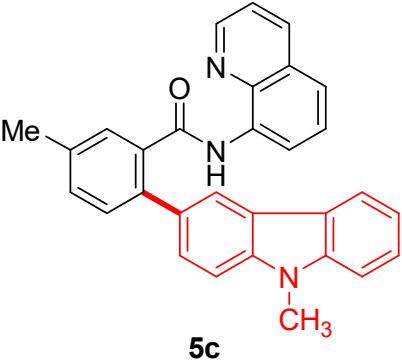


SpinWorks 4: RD-1211
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28

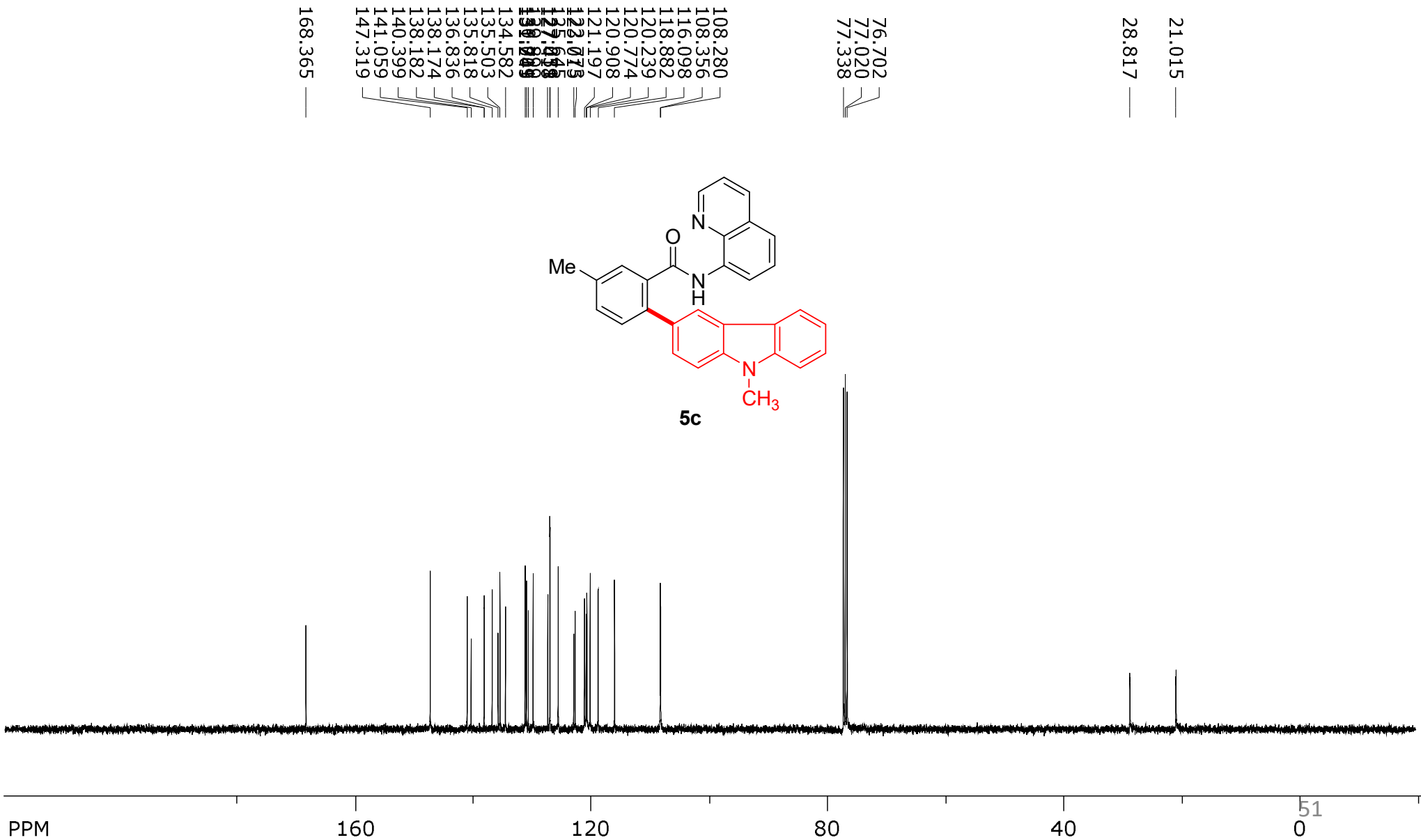


SpinWorks 4: RD-1211
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28

7.5317	7.4640	7.4413	7.4218	7.3526	7.2847	7.2360	7.1766	7.0438
7.5382	7.4710	7.4444	7.4248	7.3625	7.2732	7.2546	7.1557	7.0543
7.5509	7.4838			7.3729			7.1643	7.0642
7.5547	7.4912			7.3828				7.0734
7.5594	7.5040							
	7.5092							



SpinWorks 4: RD-1211 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



SpinWorks 4: RD-1211 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18

168.365 —

147.319 —

141.059 —

140.399 —

138.182 —

136.174 —

136.836 —

135.818 —

134.582 —

131.245 —

131.009 —

130.711 —

129.899 —

127.418 —

127.051 —

127.039 —

125.645 —

123.015 —

122.773 —

121.197 —

120.908 —

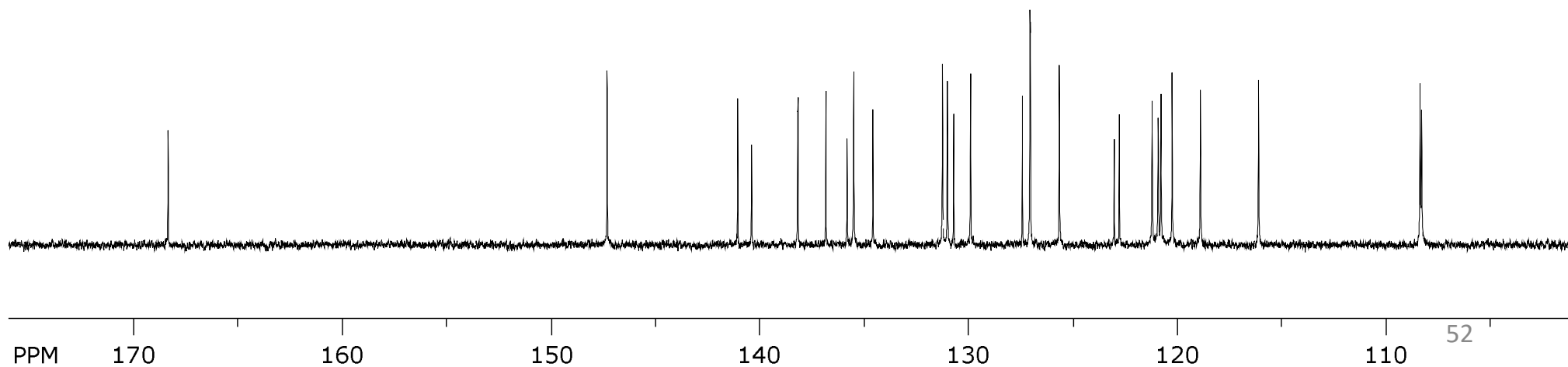
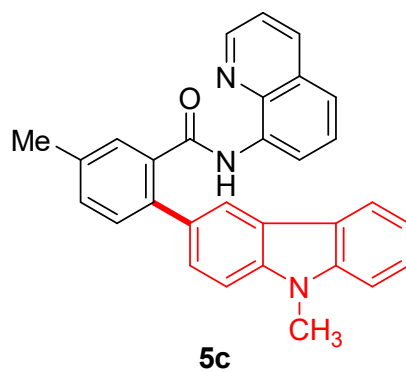
120.774 —

120.239 —

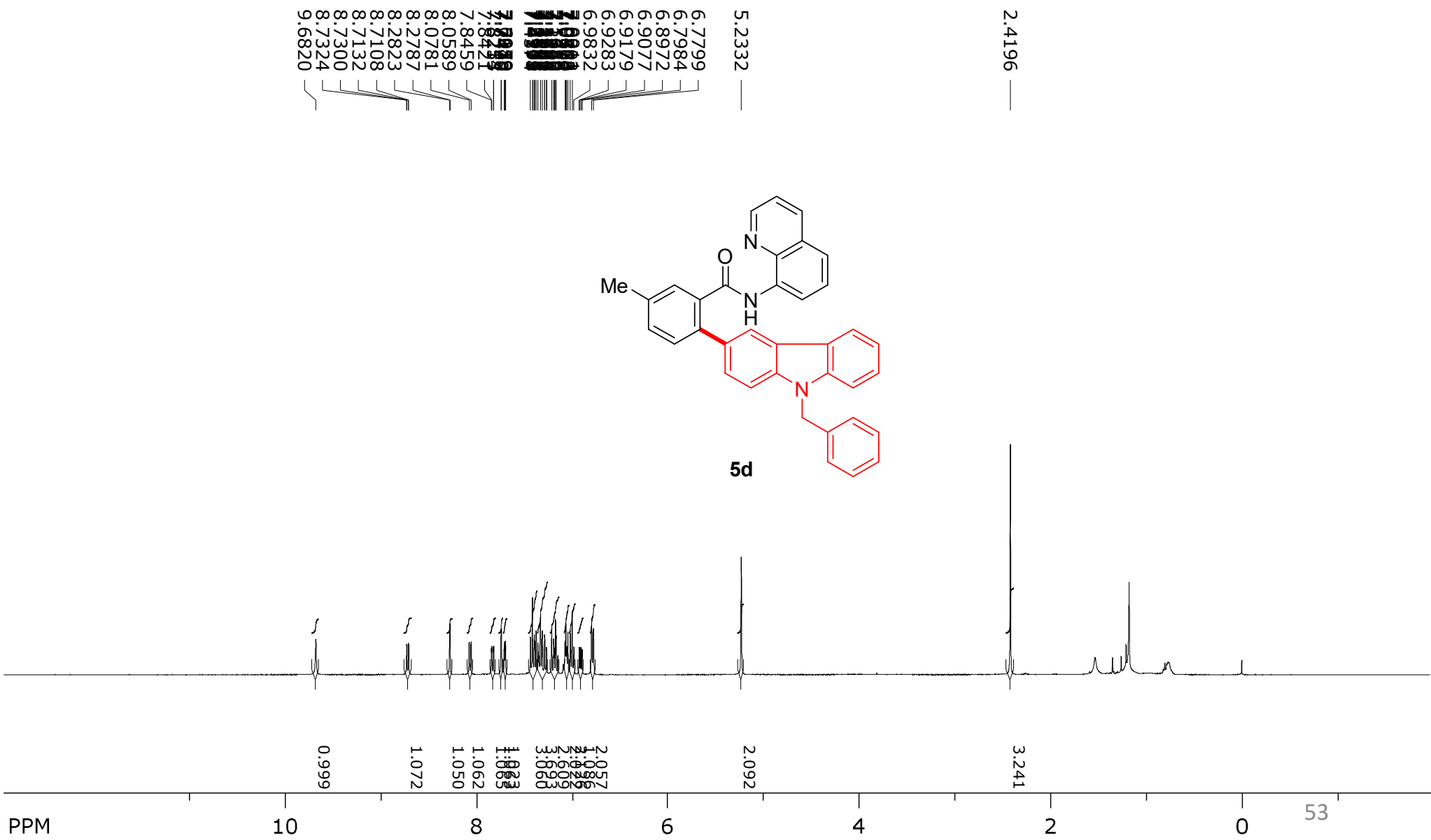
118.882 —

116.098 —

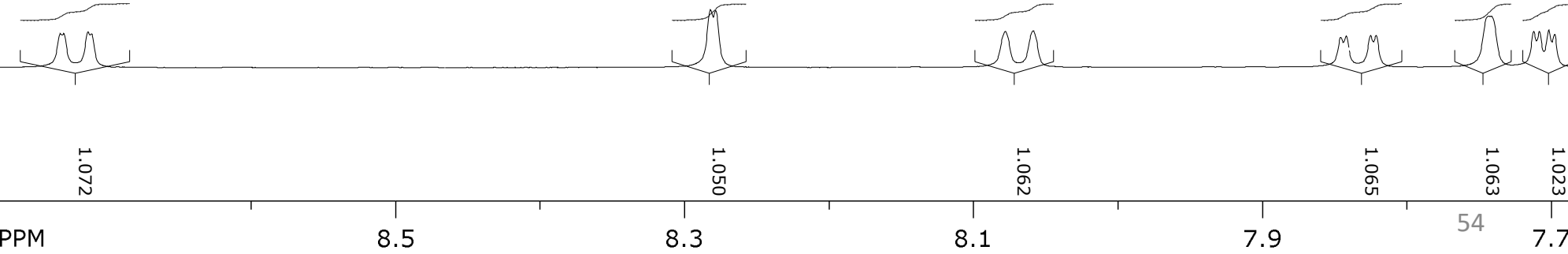
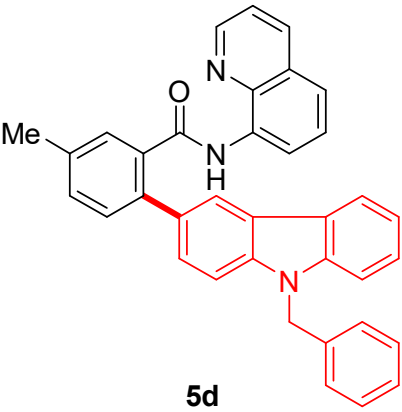
108.280 —
108.356 —



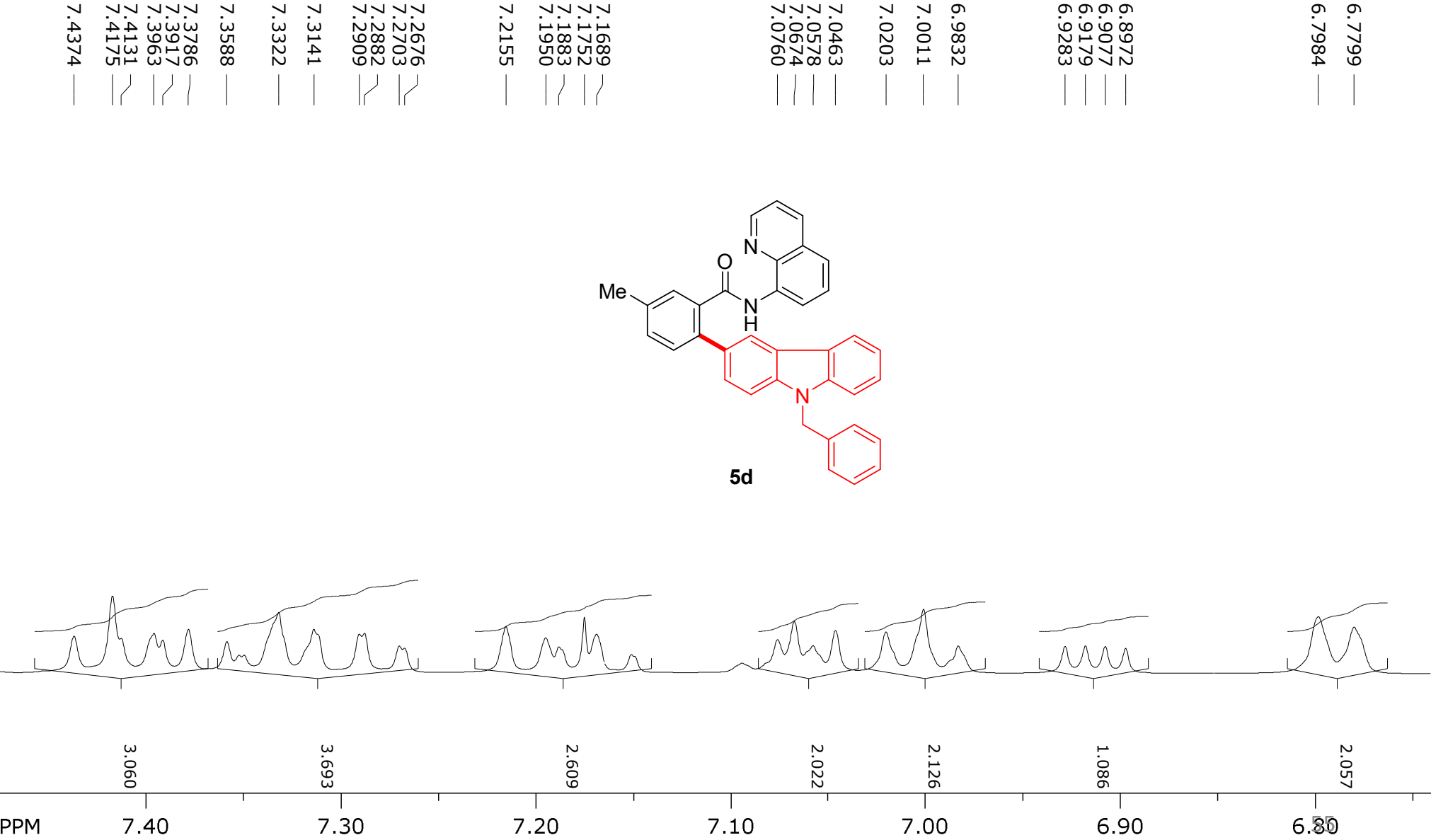
SpinWorks 4: RD-1218-Re
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56



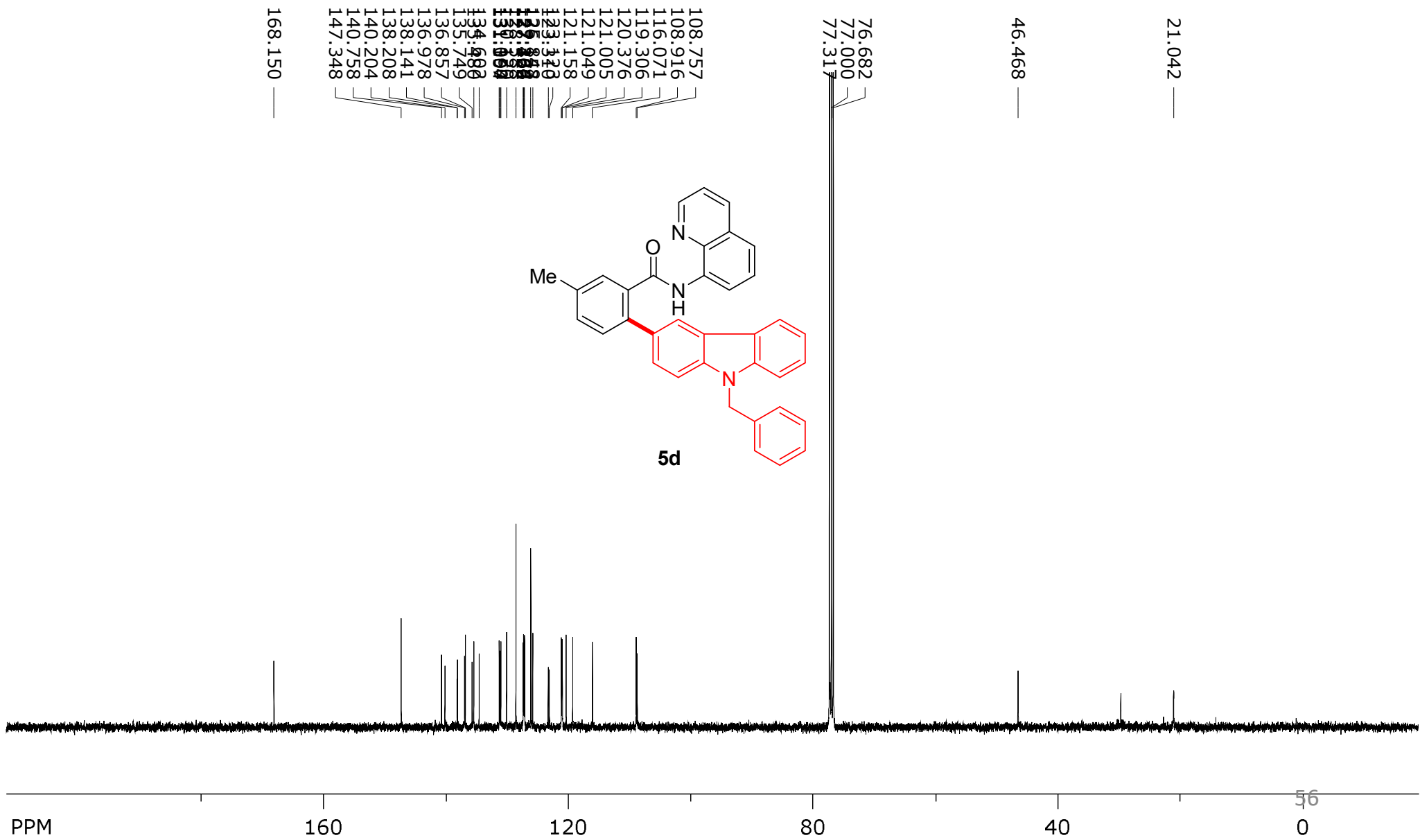
SpinWorks 4: RD-1218-Re
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56



SpinWorks 4: RD-1218-Re
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56



SpinWorks 4: RD-1218-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

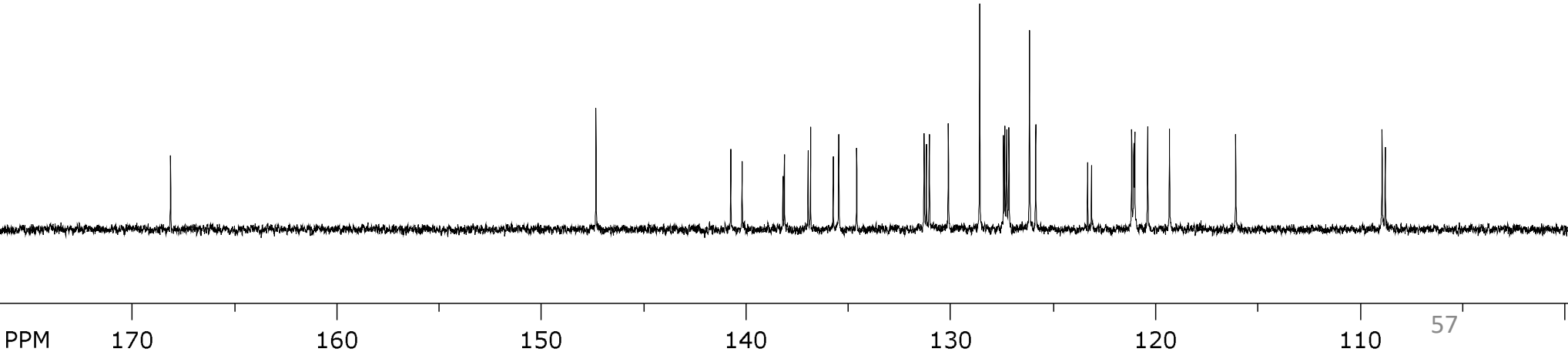
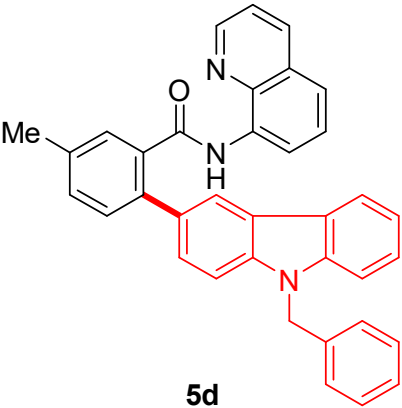


SpinWorks 4: RD-1218-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

168.150

147.348

108.757
108.916
116.071
119.306
120.376
121.005
121.049
121.158
123.123
123.310
125.848
126.153
127.164
127.266
127.362
127.422
128.588
130.120
131.050
131.197
131.304
134.602
135.480
135.749
136.857
136.978
138.141
138.208
140.204
140.758



Chemical structure of compound **5e** is shown above the spectrum. The structure is a complex molecule featuring a central benzene ring substituted with a 4-chlorobenzyl group (red), a 4-methylbenzoyl group (black), and a 1-(quinolin-2-yl)hydrazinyl group (black). The spectrum displays the ¹H NMR data for compound **5e** in CDCl₃, with the solvent peak (CDCl₃) visible at 7.26 ppm. The x-axis represents the chemical shift in PPM, ranging from 0 to 10. Integration values are provided below the baseline for each major peak group.

Chemical Shift (ppm)	Integration
~0.0	1.000
~1.3	1.154
~1.5	1.096
~1.7	1.151
~1.9	1.187
~2.1	1.167
~2.3	2.616
~2.5	1.347
~2.7	1.347
~2.9	1.347
~3.1	1.158
~3.4	2.396
~7.2	3.412



SpinWorks 4: RD 1254
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7

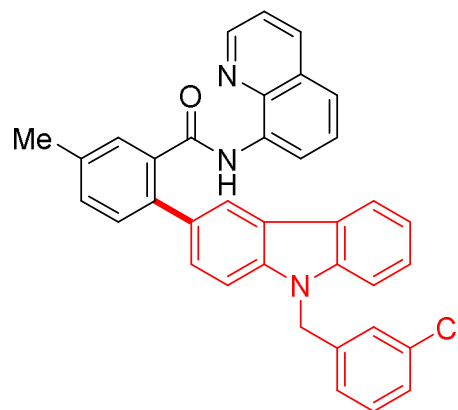
8.7773 —
8.7962 —

8.3471 —
8.3501 —

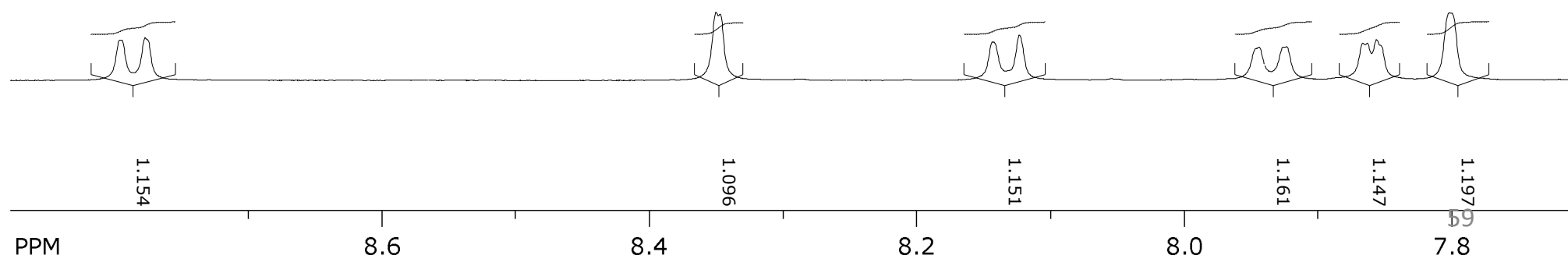
8.1231 —
8.1430 —

7.9256 —
7.9438 —

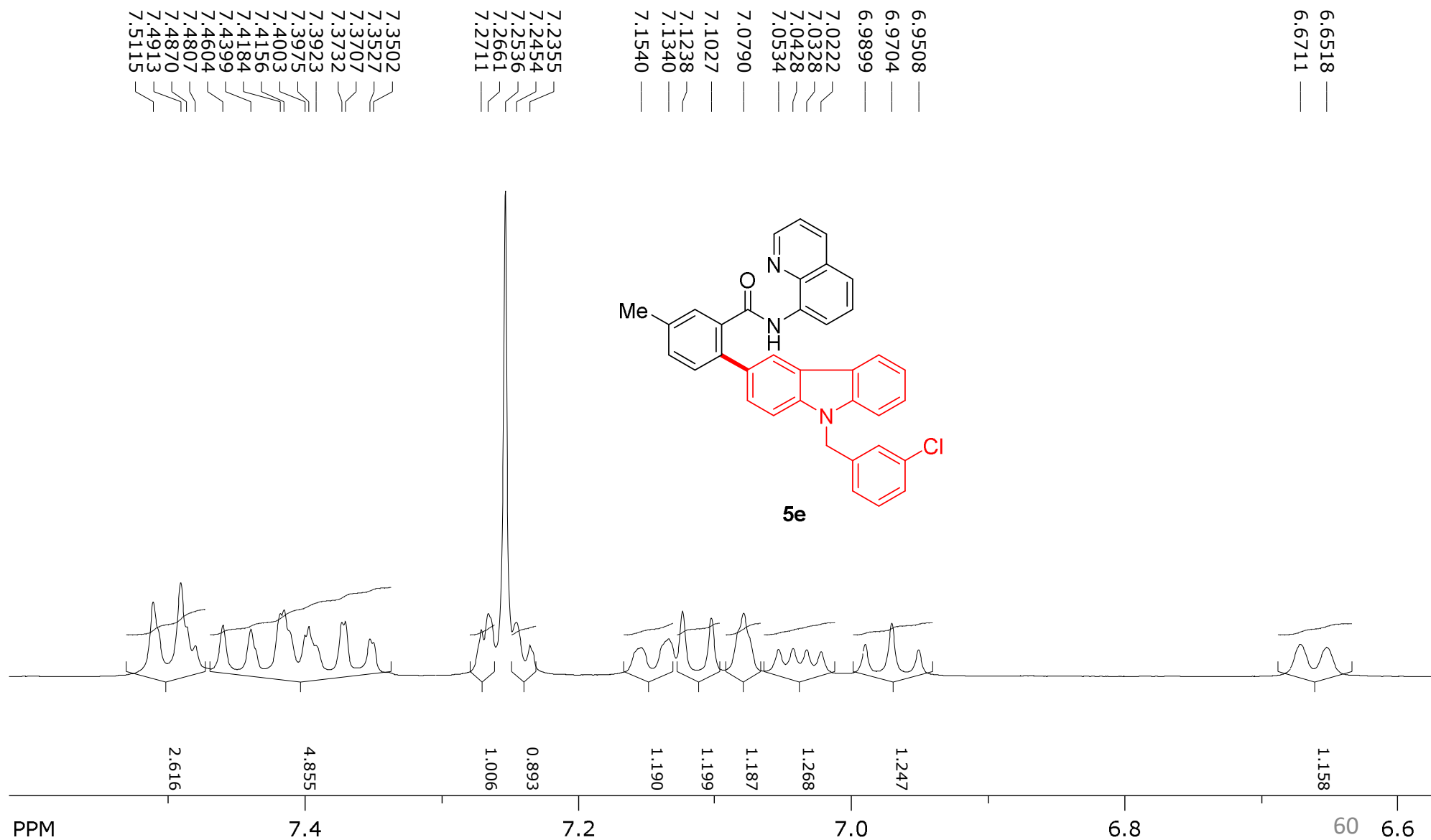
7.7996 —
7.8012 —
7.8559 —
7.8628 —
7.8662 —



5e



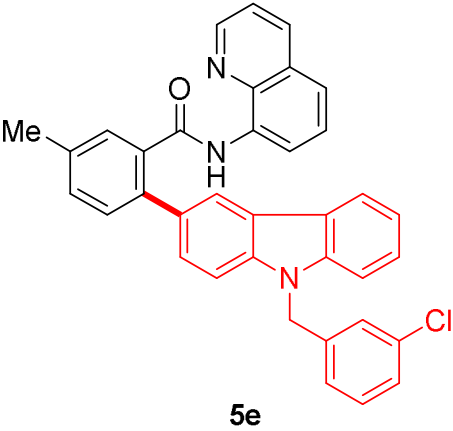
SpinWorks 4: RD 1254
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7



SpinWorks 4: RD 1254
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7

5.2626

2.4961



2.396

3.412

PPM 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 61 2.0

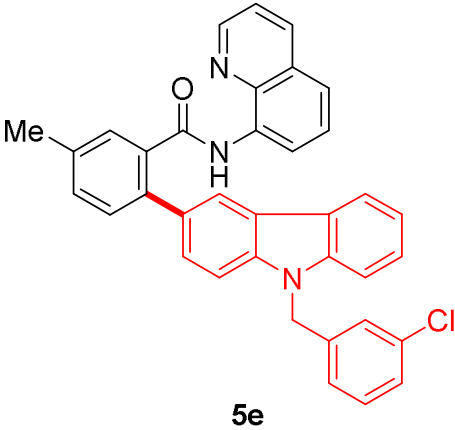
SpinWorks 4: RD-1254
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

108.5326
108.7065
116.2347
119.4879
120.3948
120.9765
121.2270
123.1013
123.3189
124.3000
125.8000
131.8000
131.8000
134.4846
135.6846
135.7299
136.9536
137.9601
137.9967
138.9698
139.9394
140.5689
147.1971
168.1705

76.6826
77.0000
77.3181

45.9270

20.9864



PPM

160

120

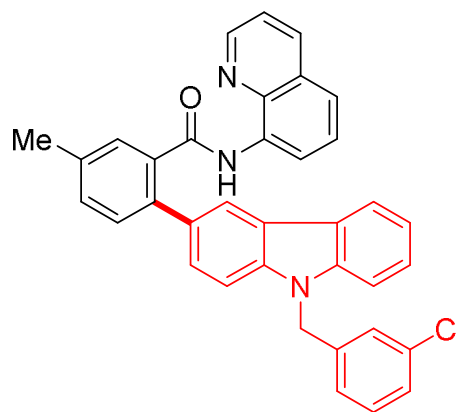
80

40

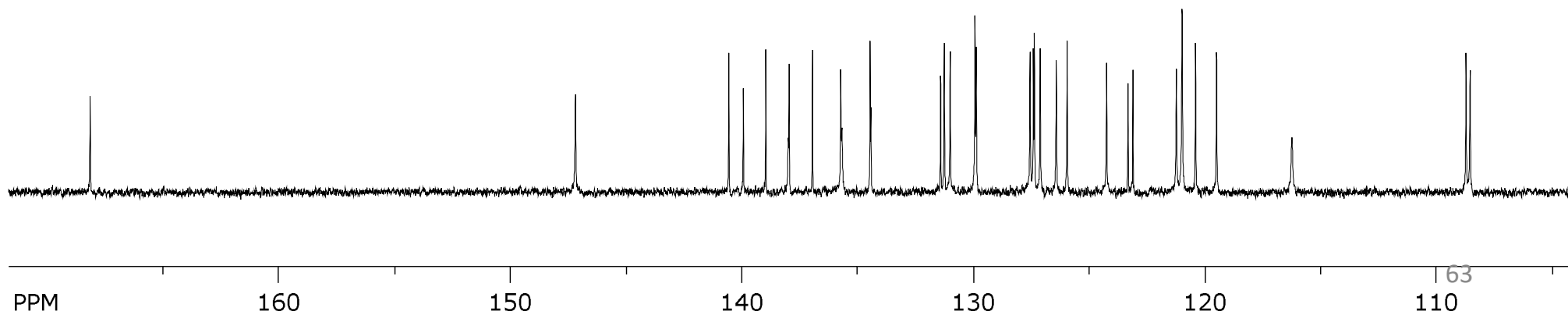
0

SpinWorks 4: RD-1254
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

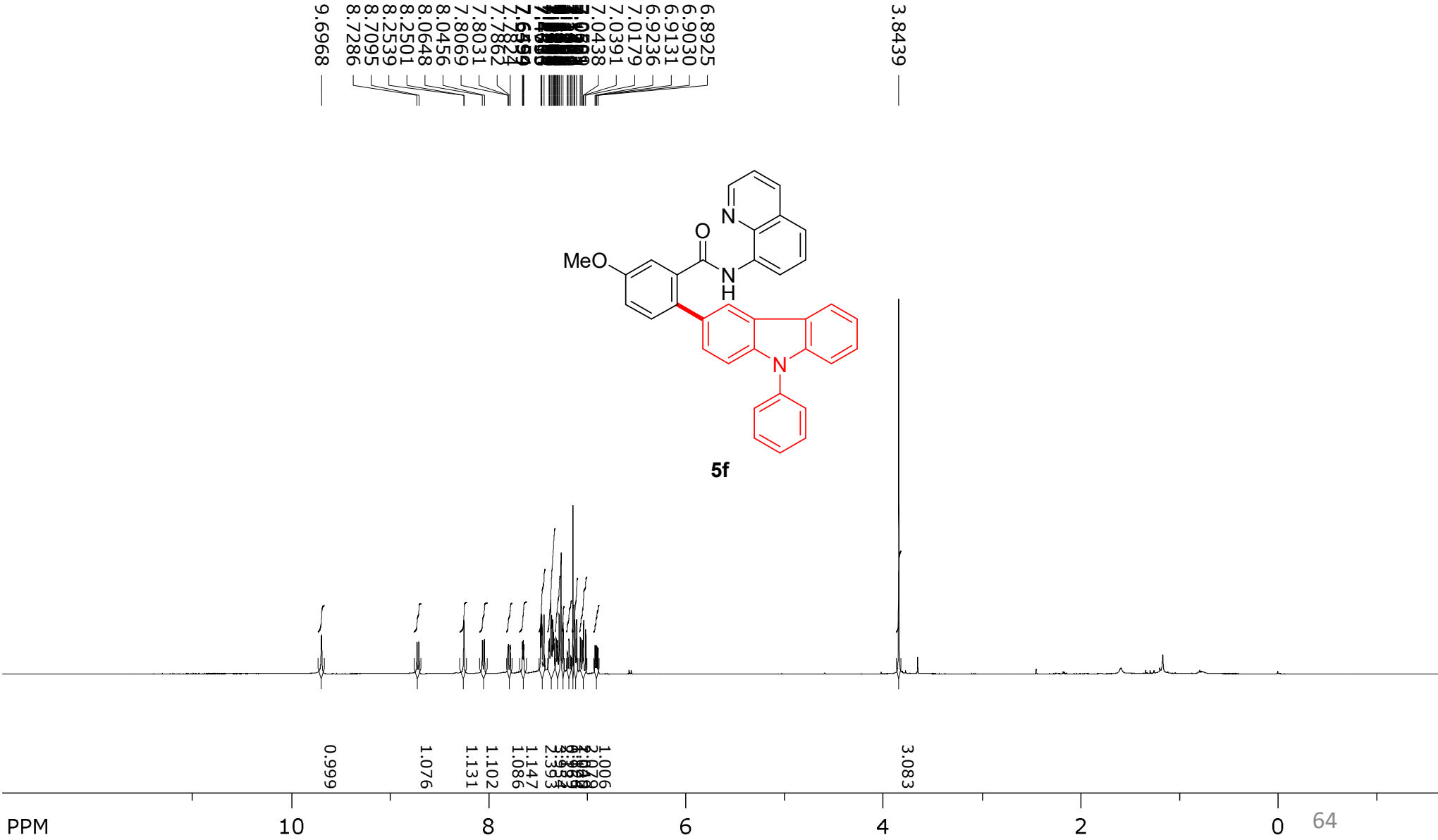
108.5326
108.7065
116.2347
119.4879
120.3948
120.9765
121.2270
123.1013
123.3180
124.2427
125.9502
126.4186
127.1103
127.3653
127.4094
127.5468
129.8764
129.9309
131.0034
131.2552
131.4163
134.4276
134.4614
135.6846
135.7299
136.9536
137.9601
137.9967
138.9698
139.9394
140.5689
147.1971
168.1705



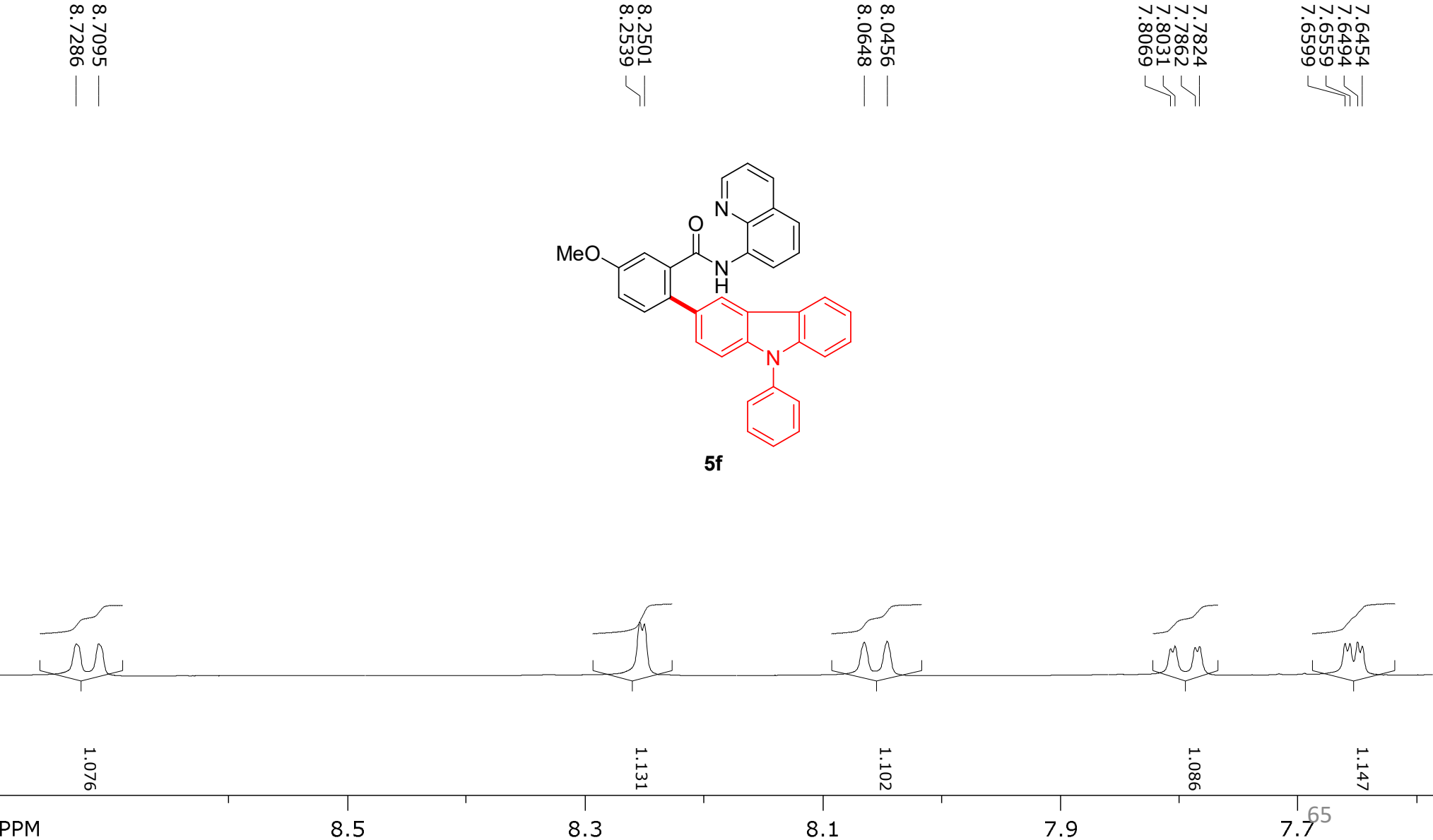
5e



SpinWorks 4: RD-1215
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

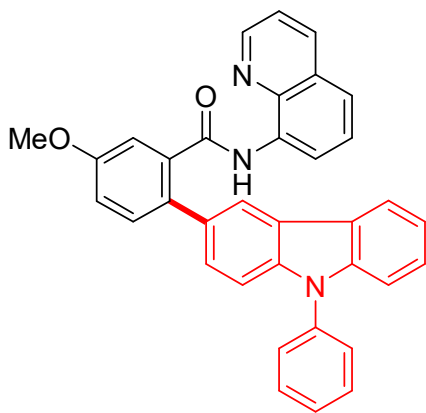


SpinWorks 4: RD-1215
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

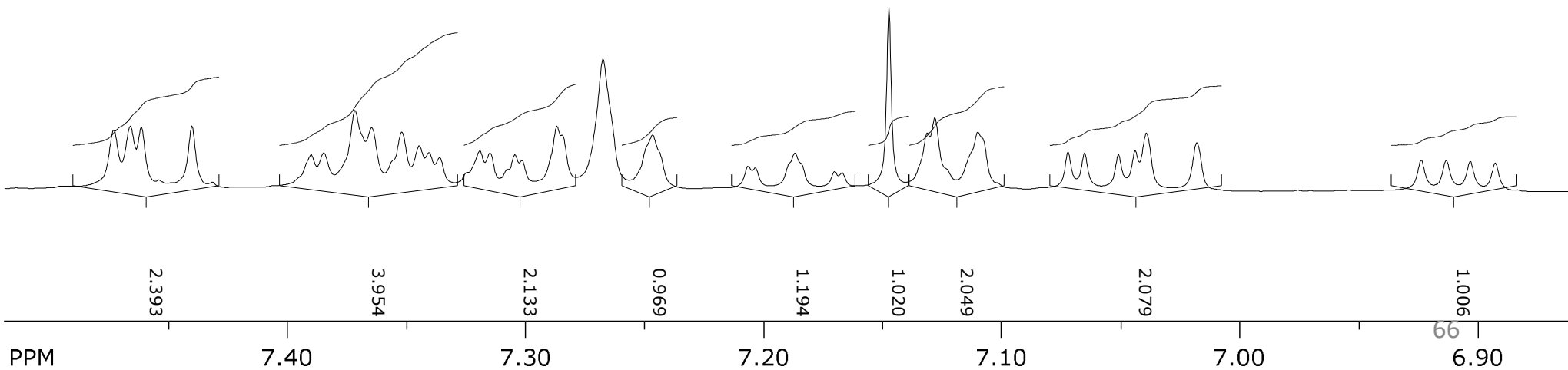


SpinWorks 4: RD-1215
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

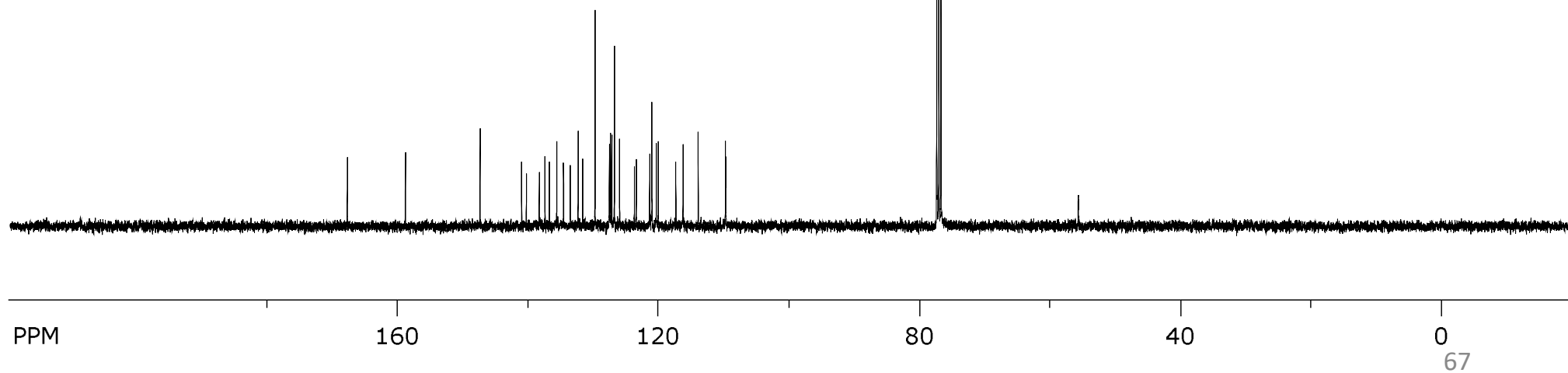
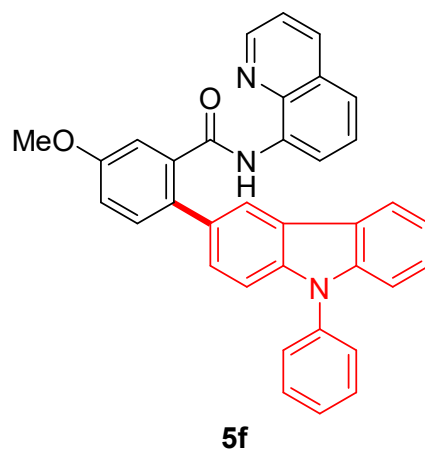
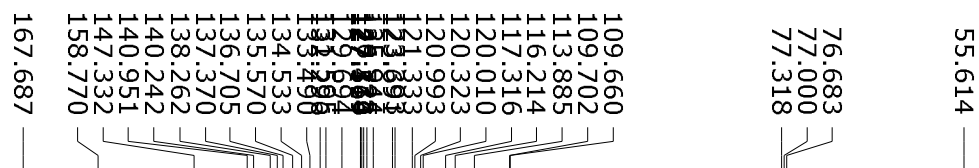
7.4616	7.4404	7.3903	7.3850	7.3718	7.3648	7.3522	7.3448	7.3407	7.3363	7.3247	7.3194	7.3151	7.3077	7.3046	7.3016	7.2870	7.2848	7.2676	7.2467	7.2036	7.1869	7.1702	7.1671	7.1473	7.1313	7.1281	7.1101	7.0721	7.0651	7.0509	7.0438	7.0391	7.0179	6.9236	6.9131	6.9030	6.8925			
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	
7.4733	7.4663	7.4533	7.4403	7.4273	7.4143	7.4013	7.3883	7.3753	7.3623	7.3493	7.3363	7.3233	7.3103	7.2973	7.2843	7.2713	7.2583	7.2453	7.2323	7.2193	7.2063	7.1933	7.1803	7.1673	7.1543	7.1413	7.1283	7.1153	7.1023	7.0893	7.0763	7.0633	7.0503	7.0373	7.0243	7.0113	6.9983	6.9853	6.9723	6.9593



5f

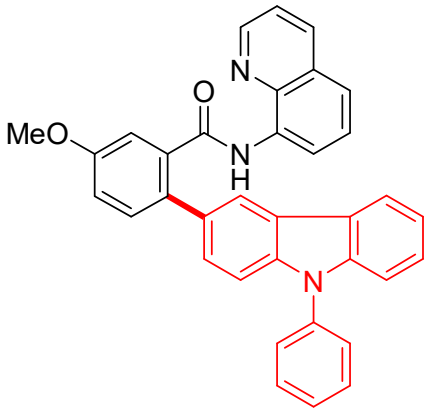


C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

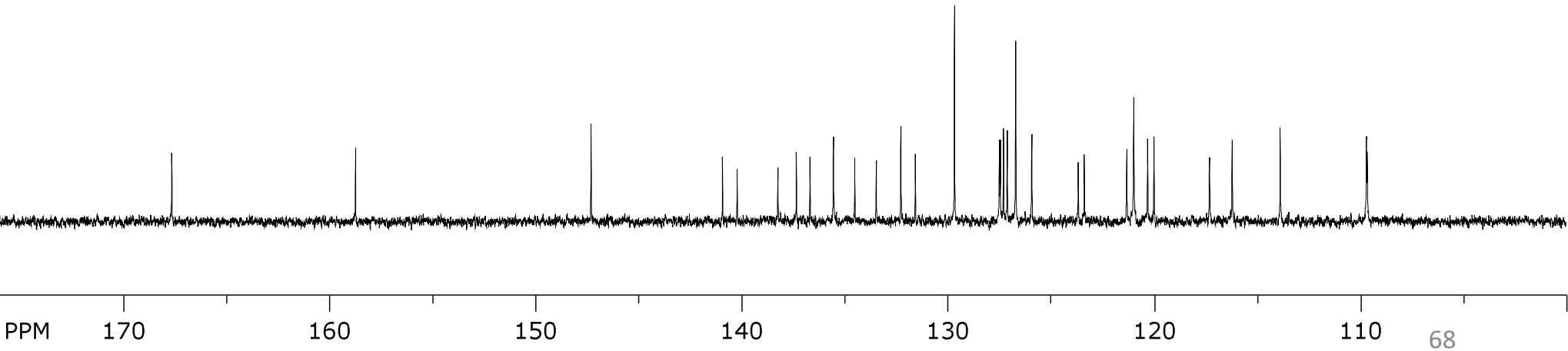


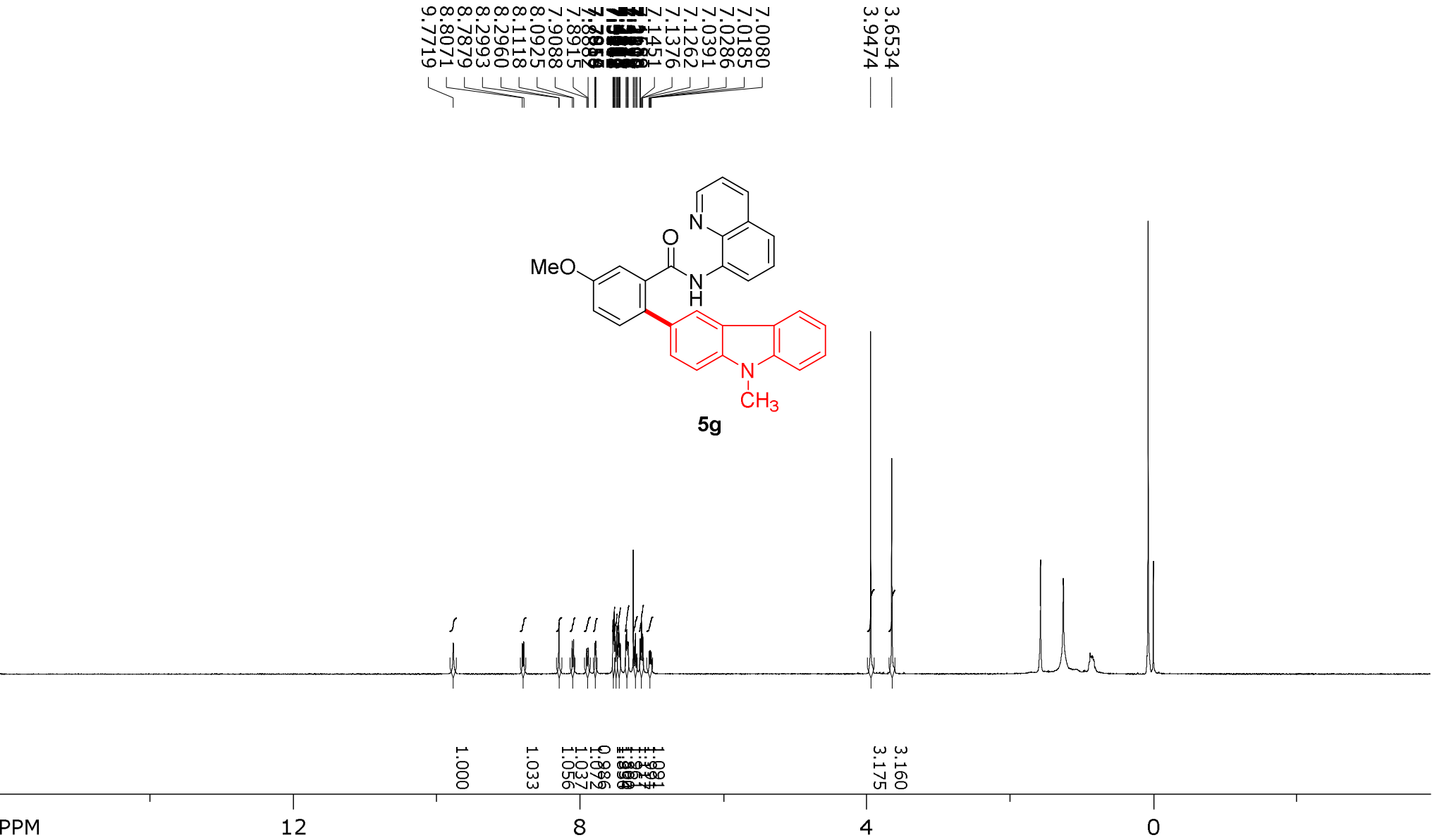
SpinWorks 4: RD-1215
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

167.687 —
158.770 —
147.332 —
140.242 —
140.951 —
138.262 —
137.370 —
136.705 —
135.570 —
134.533 —
133.490 —
132.296 —
131.595 —
129.694 —
127.514 —
127.469 —
127.316 —
127.133 —
126.725 —
125.944 —
123.691 —
123.393 —
121.333 —
120.993 —
120.323 —
120.010 —
117.316 —
116.214 —
113.885 —
109.660 —
109.702 —

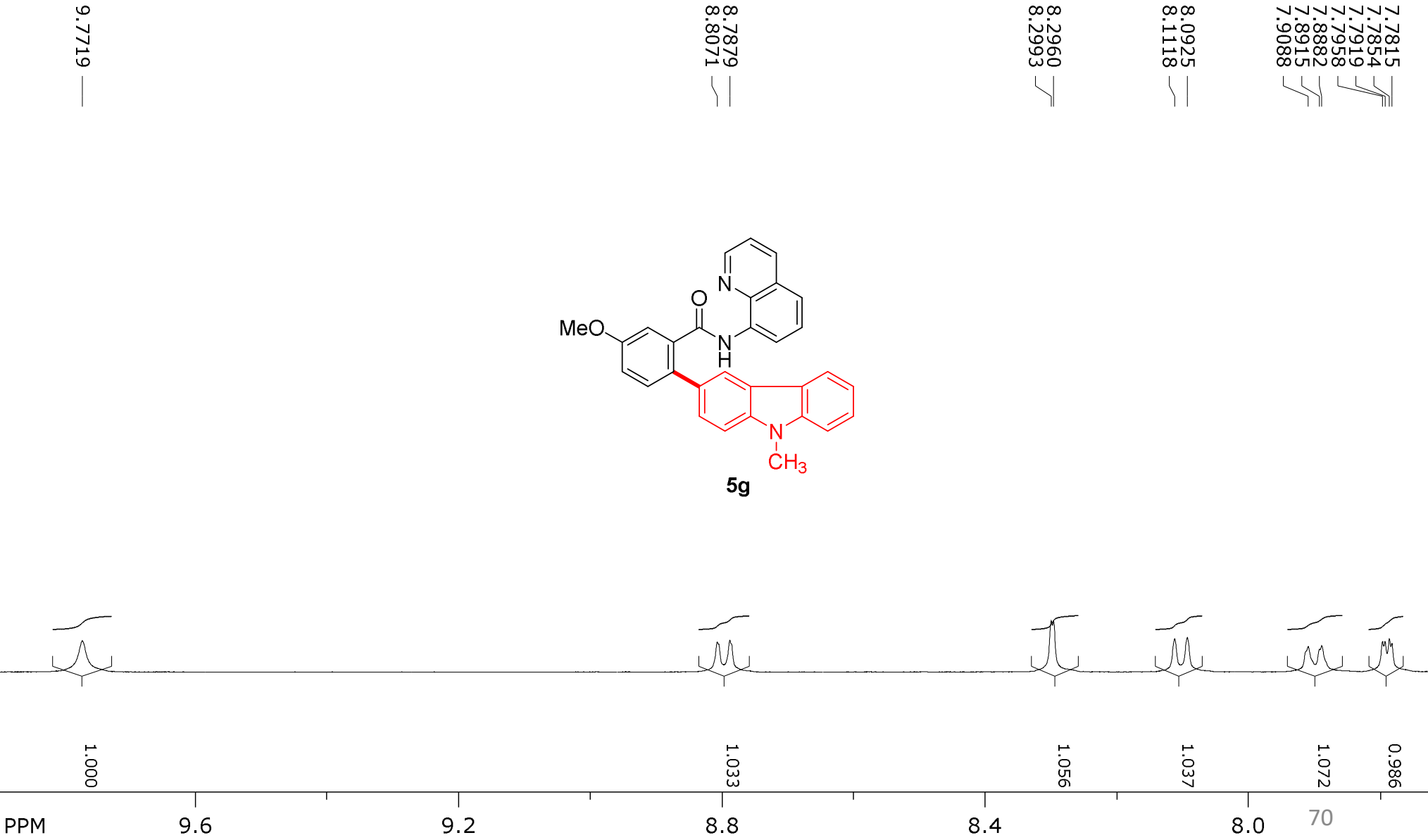


5f

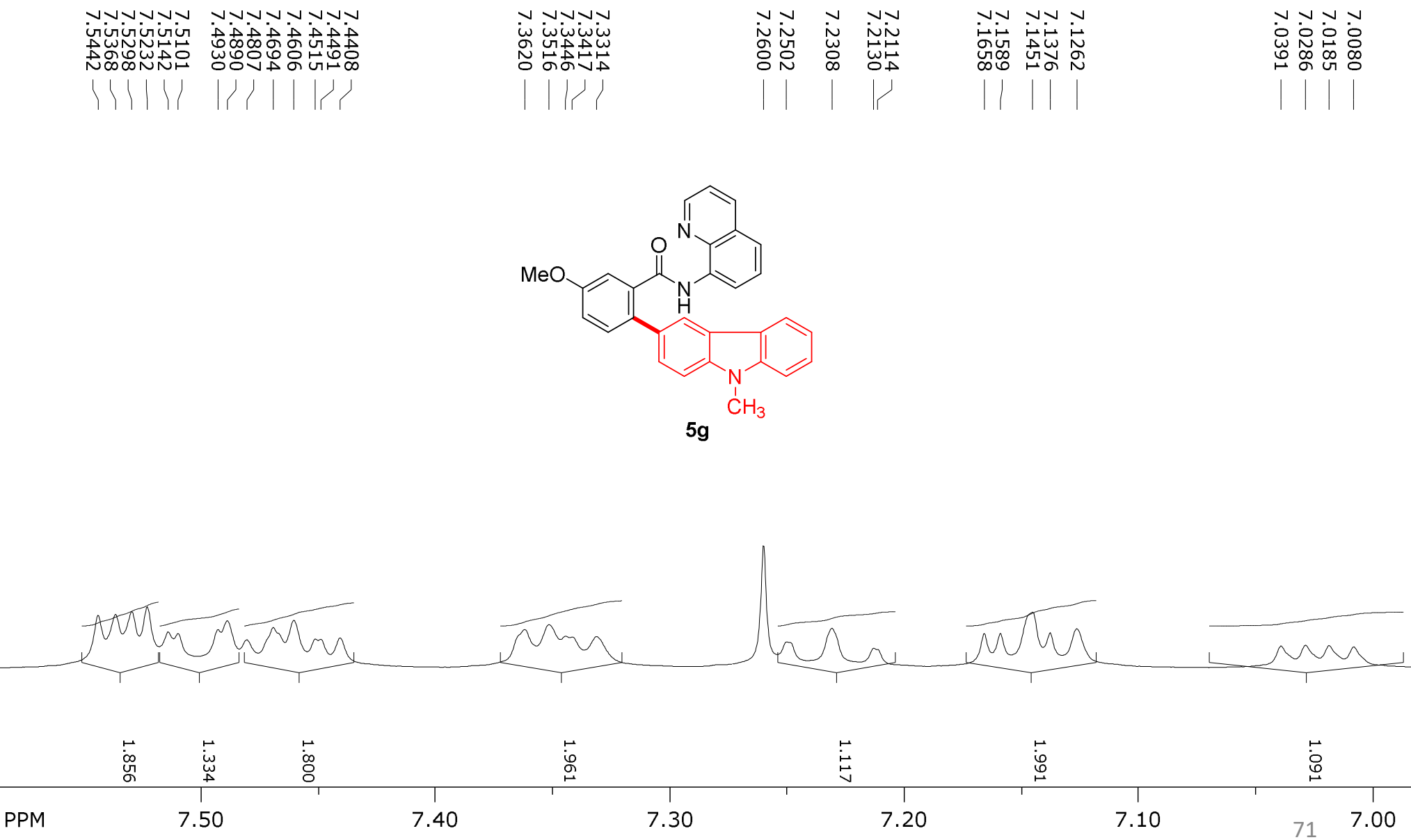




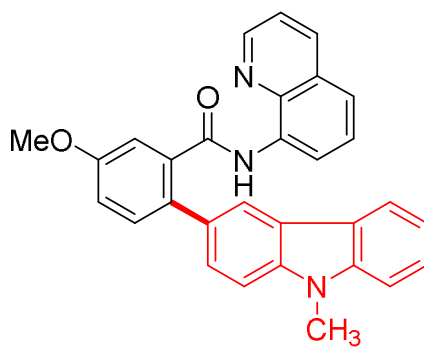
SpinWorks 4: RD-735



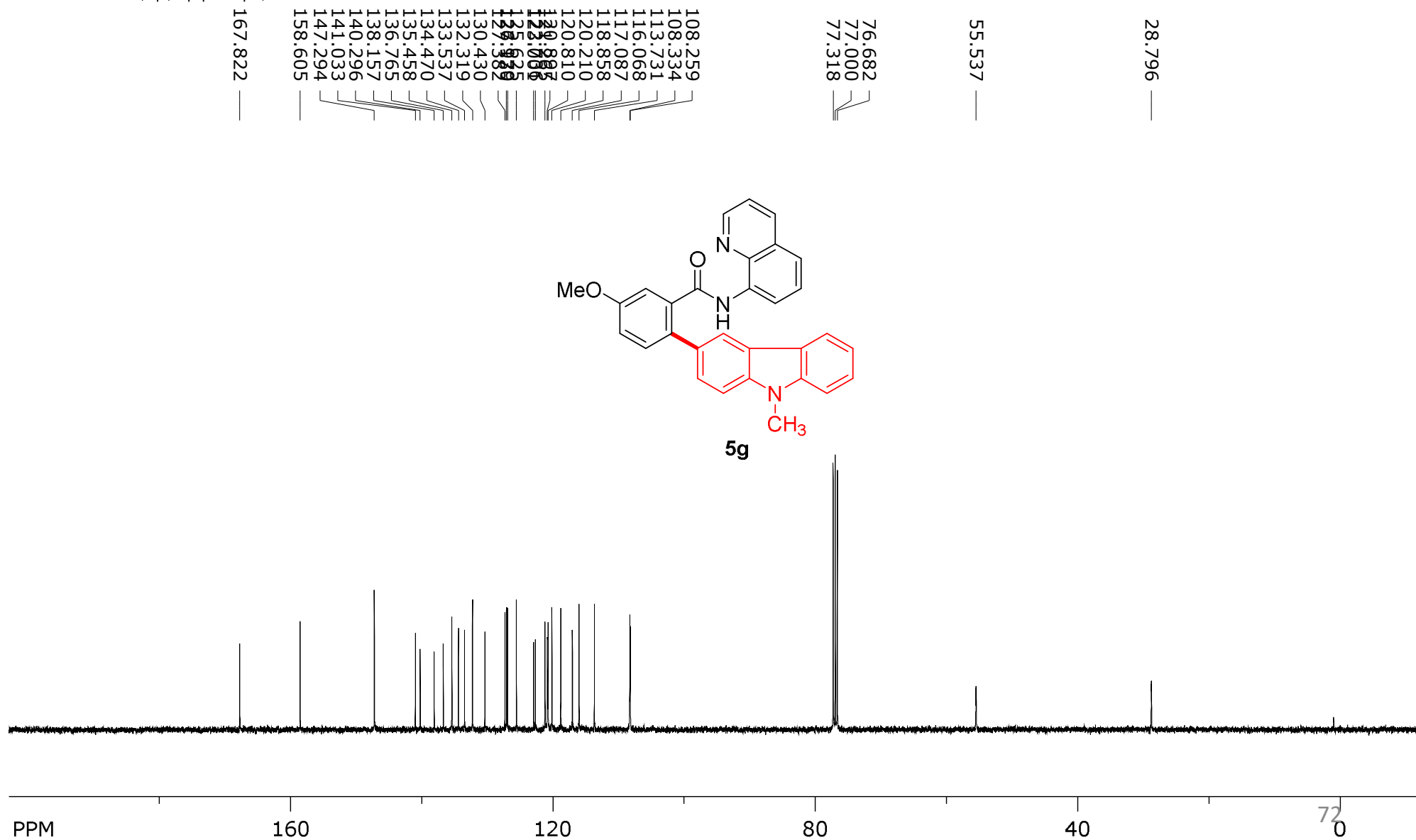
SpinWorks 4: RD-735



SpinWorks 4: RD 735
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

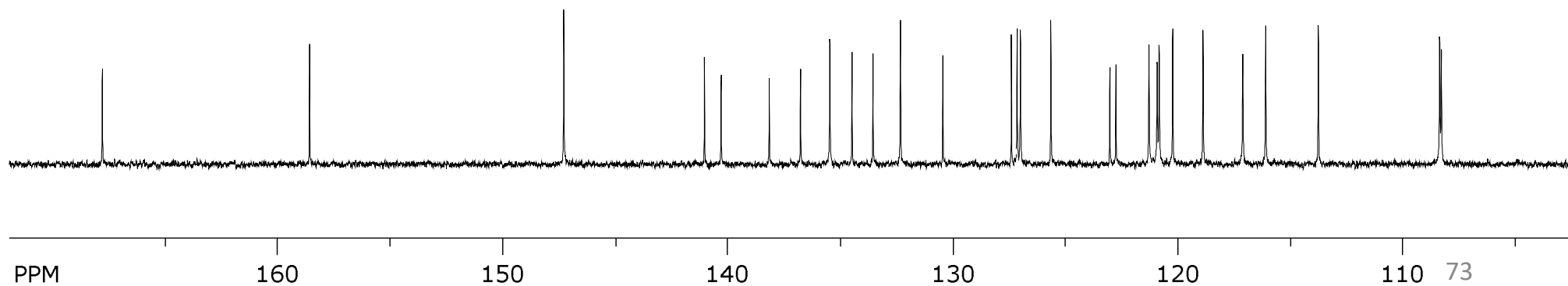
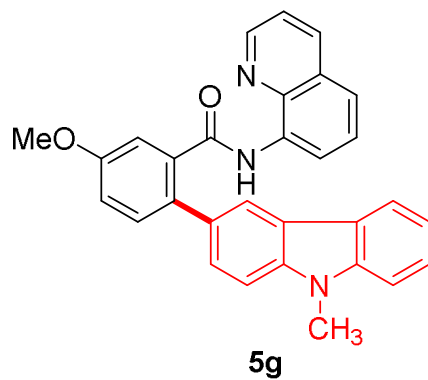


5g

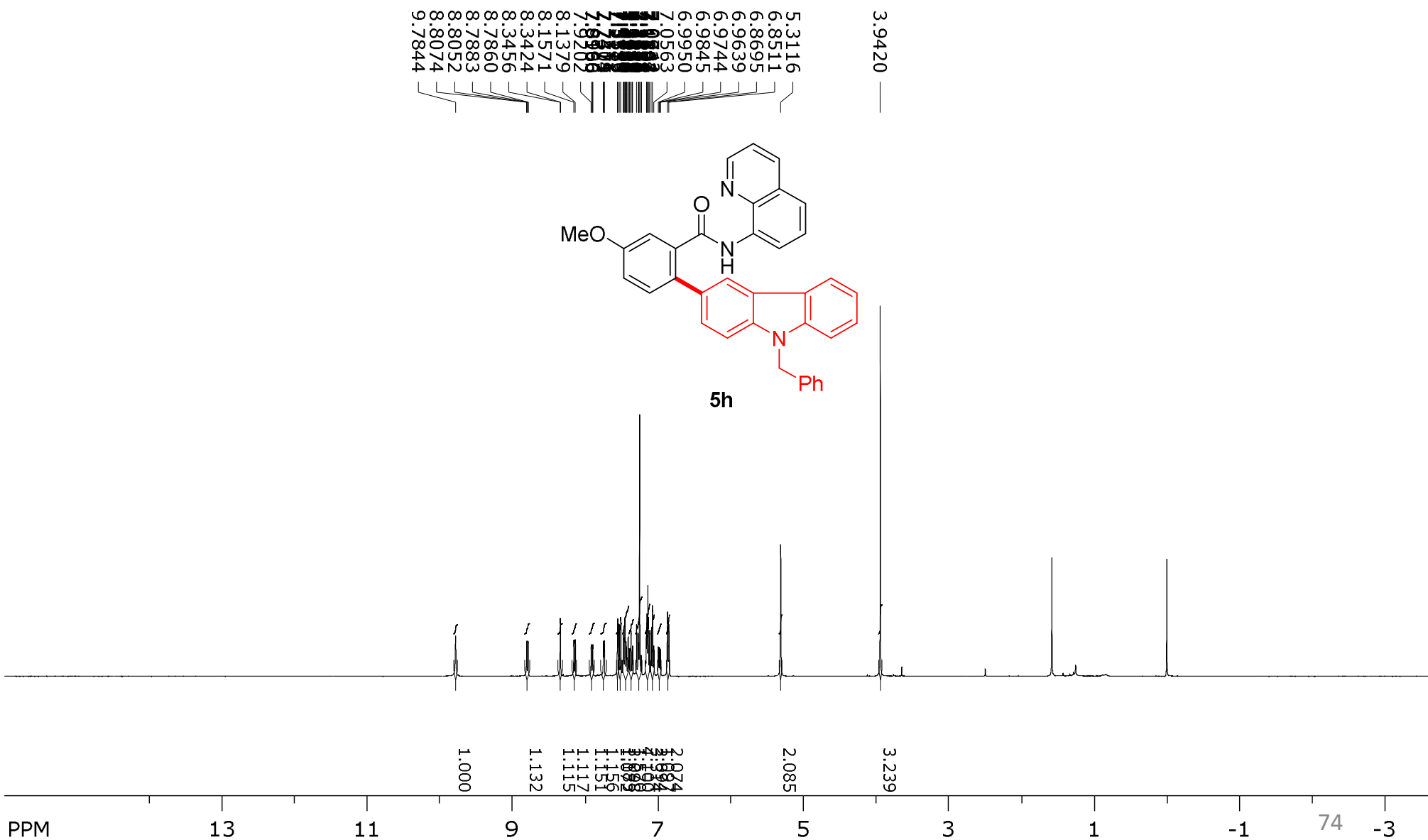


SpinWorks 4: RD 735
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

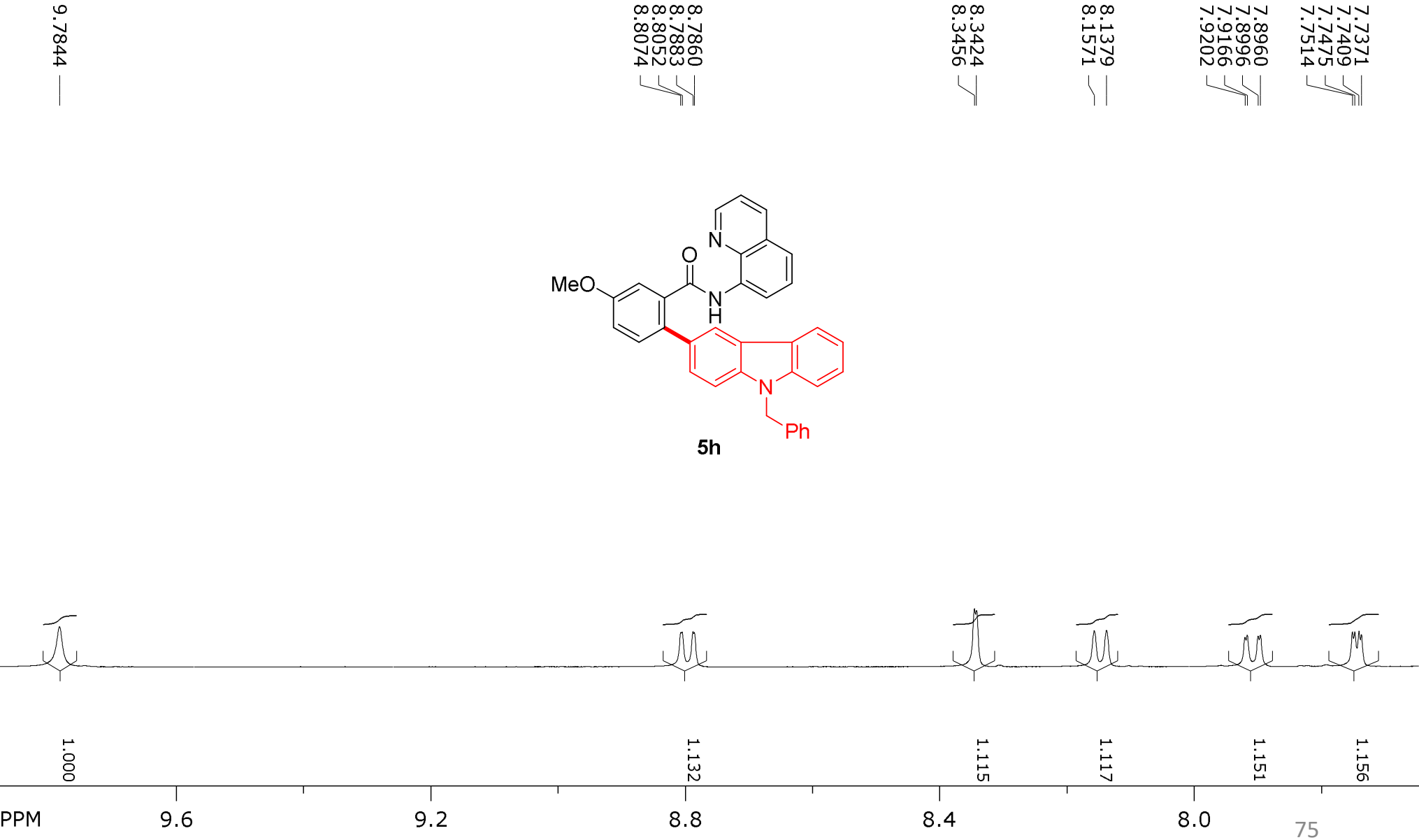
167.822 —
158.605 —
147.294 —
140.296 —
141.033 —
138.157 —
136.765 —
135.458 —
134.470 —
133.537 —
132.319 —
130.430 —
127.382 —
127.130 —
126.979 —
125.625 —
123.001 —
122.736 —
121.265 —
120.897 —
120.810 —
120.210 —
118.858 —
117.087 —
116.068 —
113.731 —
108.334 —
108.259 —



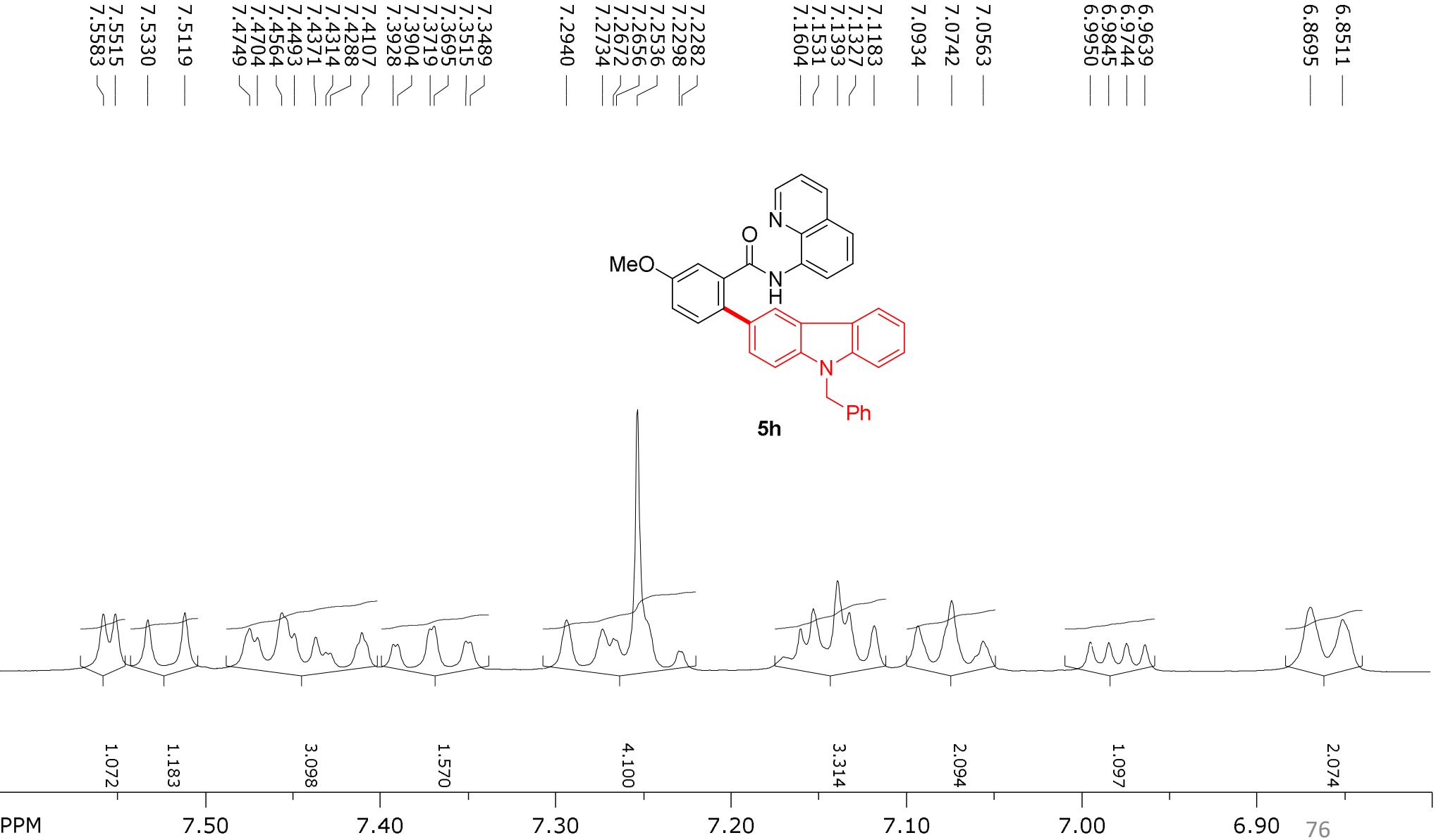
PPM



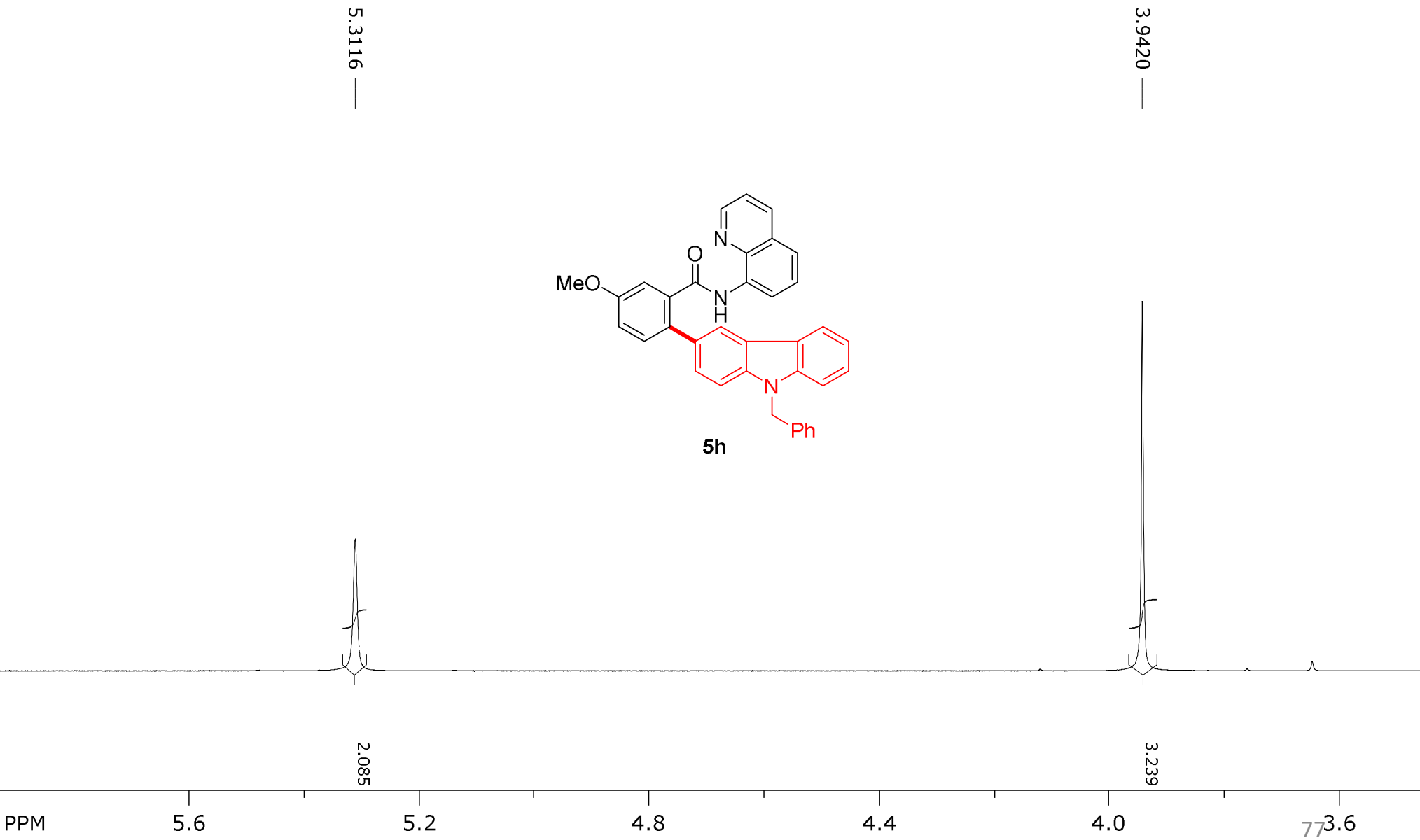
SpinWorks 4: RD-1235-RE-1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



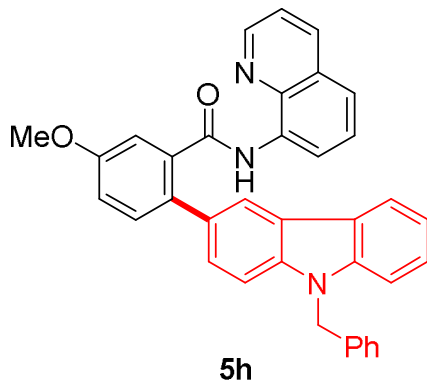
SpinWorks 4: RD-1235-RE-1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



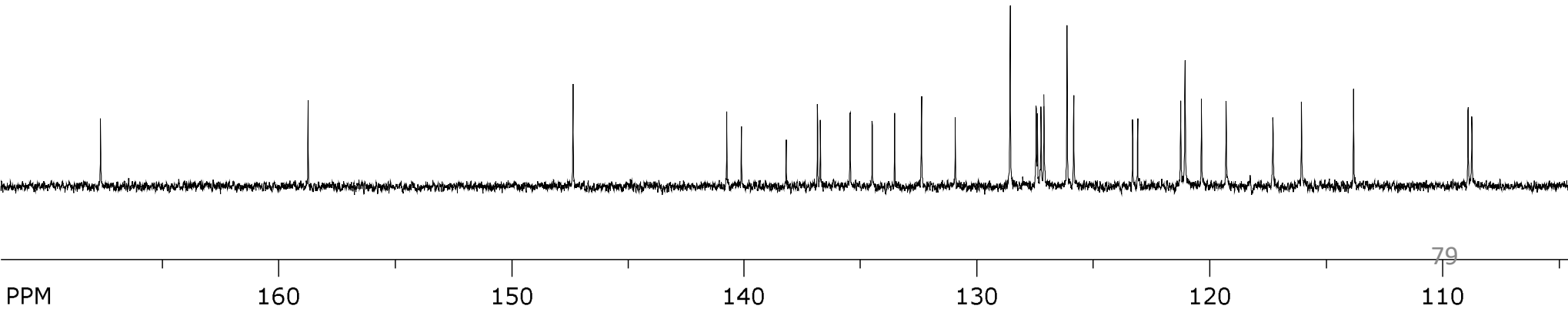
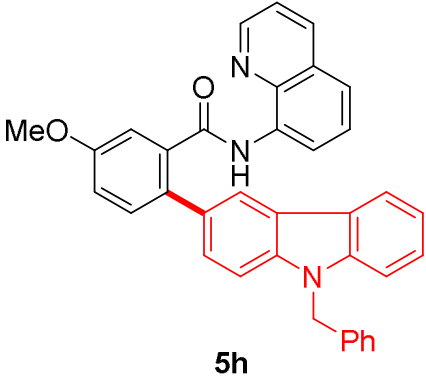
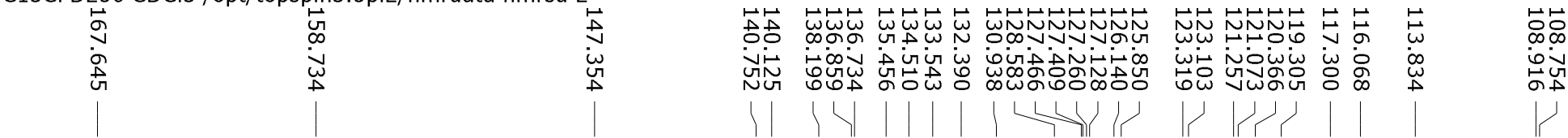
SpinWorks 4: RD-1235-RE-1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

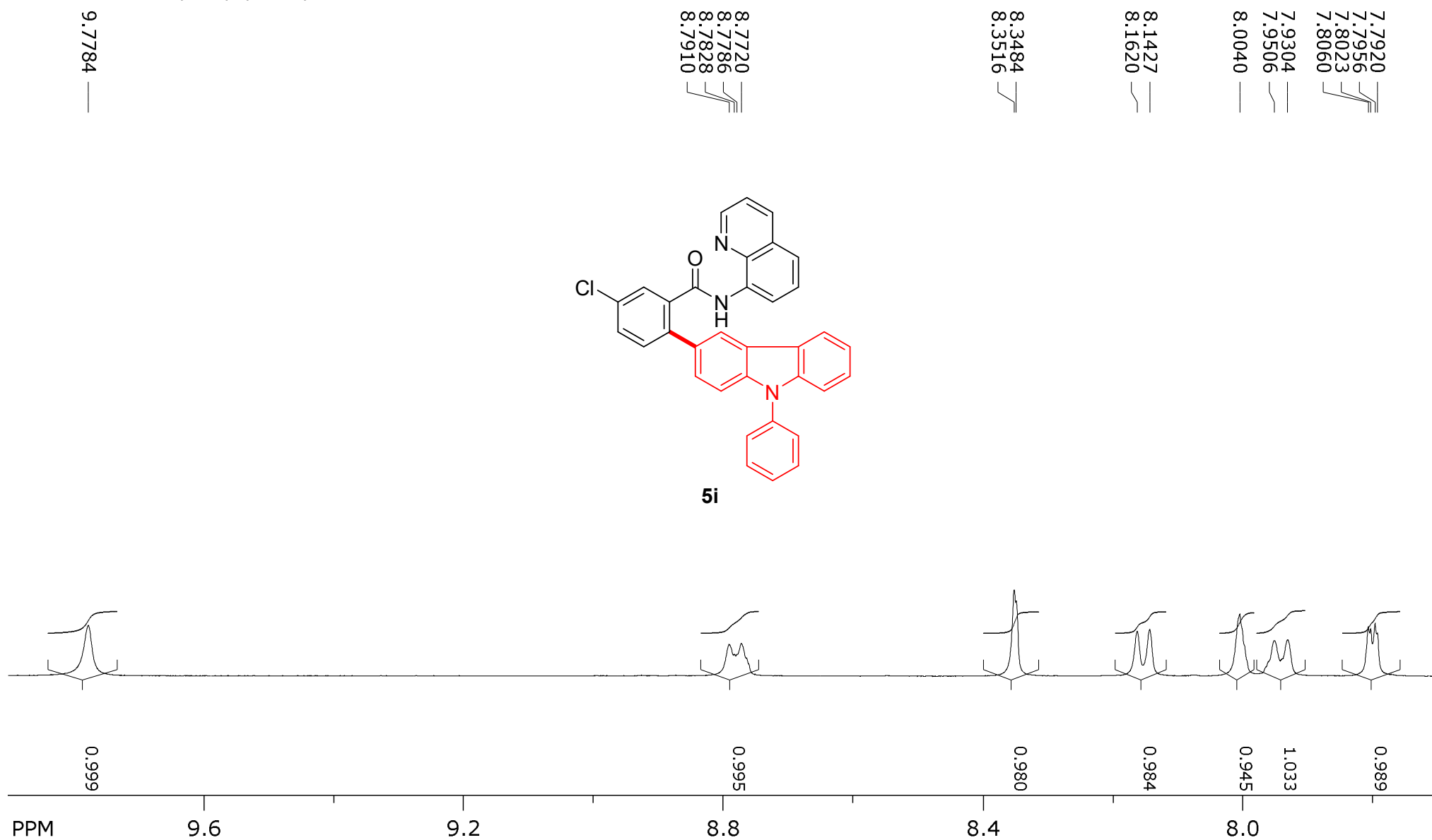


SpinWorks 4: RD-1235
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

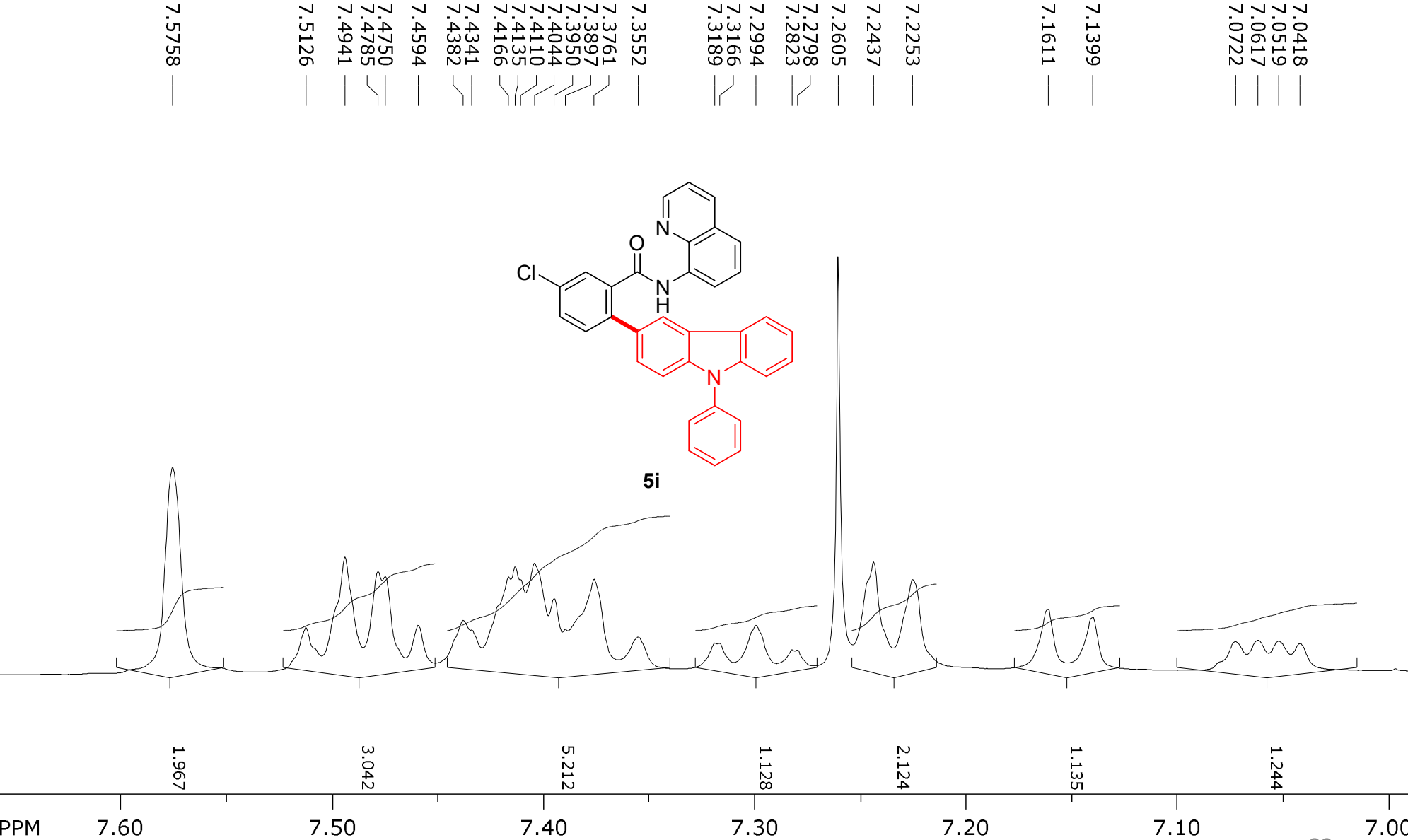


[illegible]

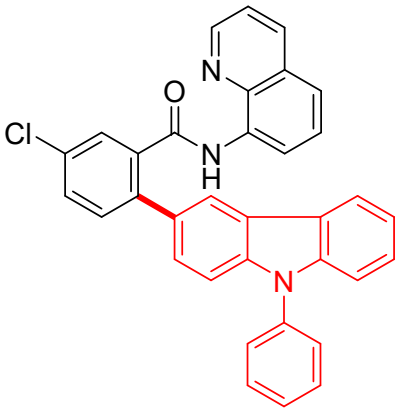
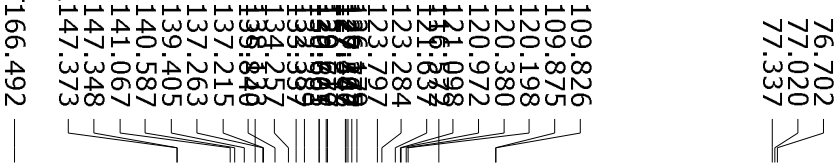
SpinWorks 4: RD-1252-Re
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5



SpinWorks 4: RD-1252-Re
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5



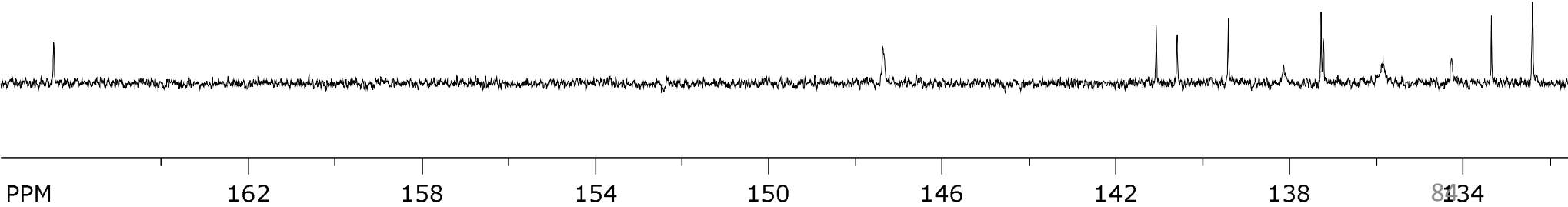
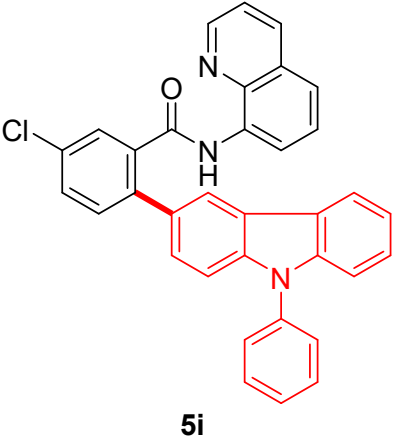
SpinWorks 4: RD-1252
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12



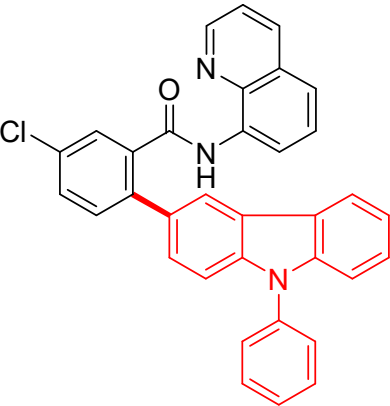
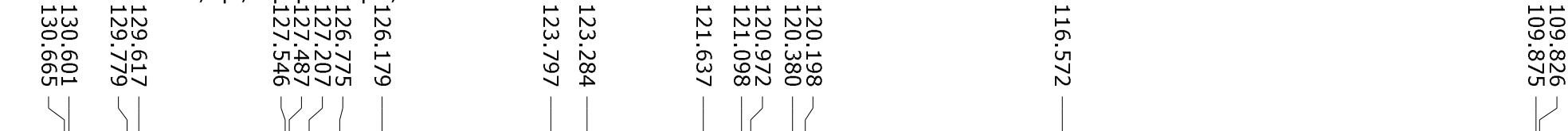
5i



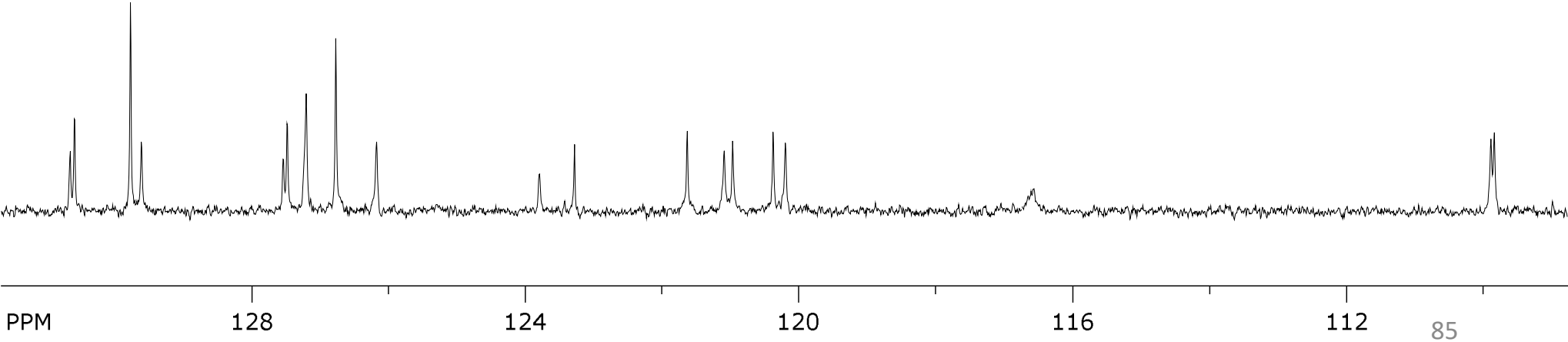
SpinWorks 4: RD-1252
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12



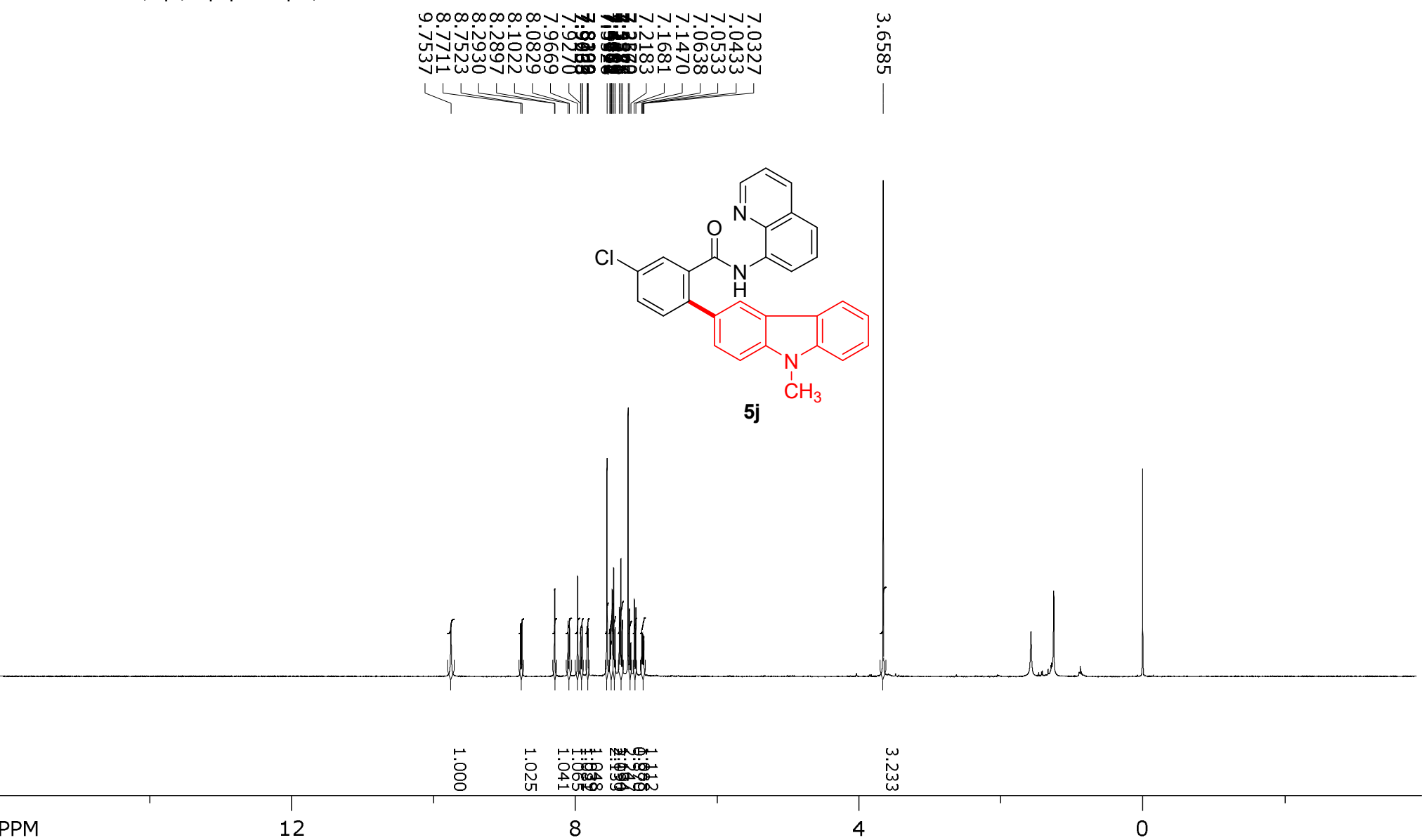
SpinWorks 4: RD-1252
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12



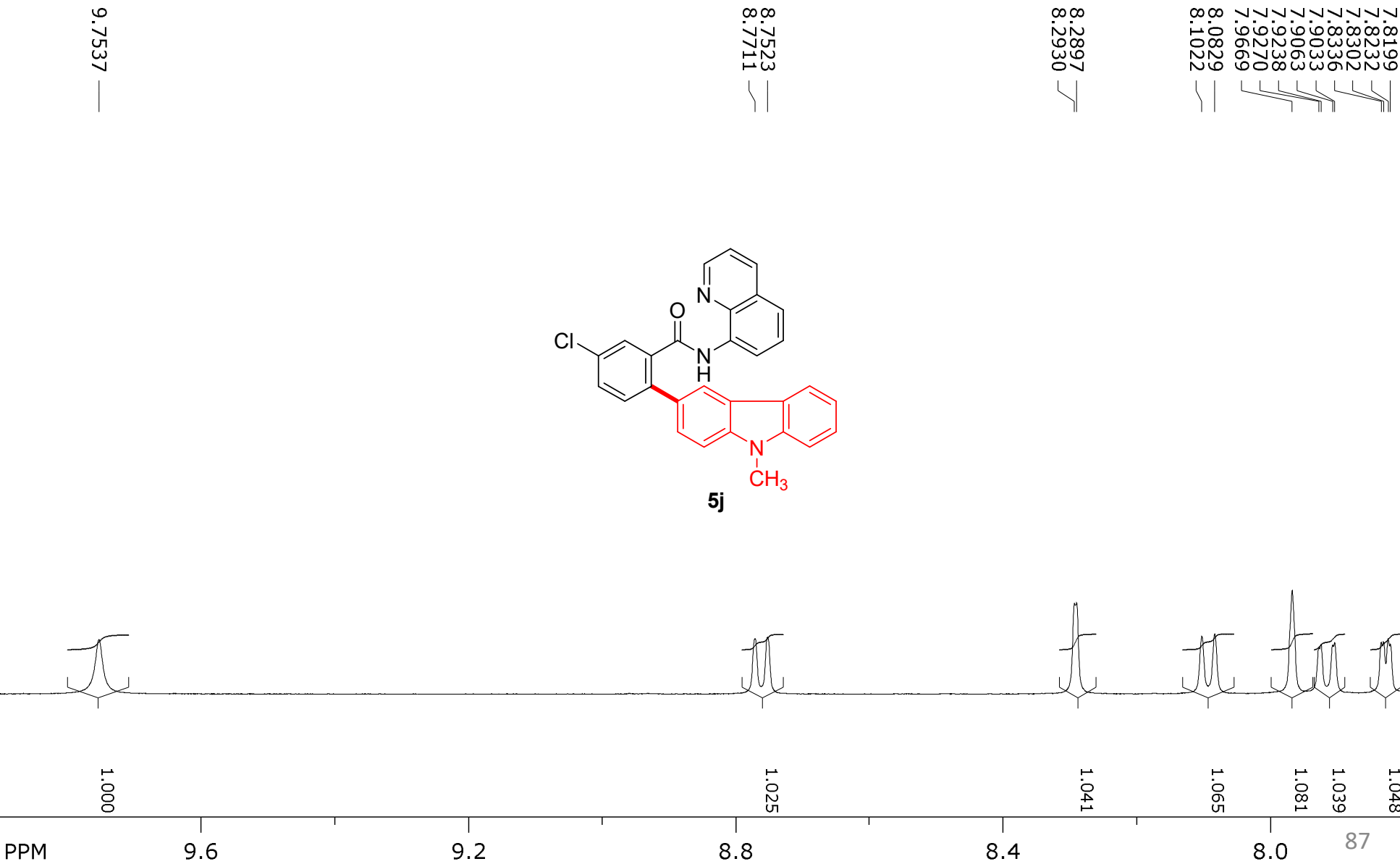
5i



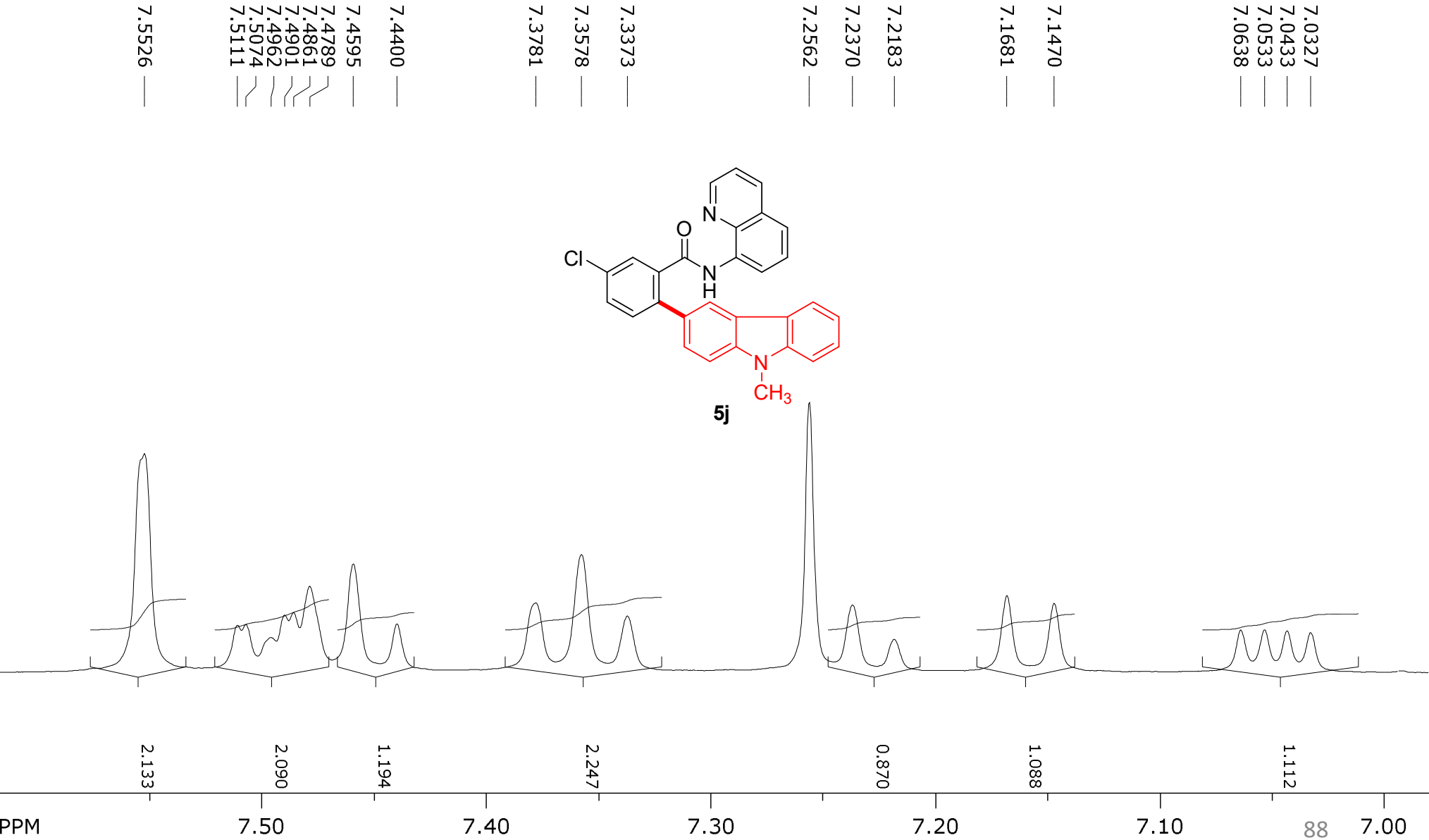
SpinWorks 4: RD 890
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



SpinWorks 4: RD 890
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



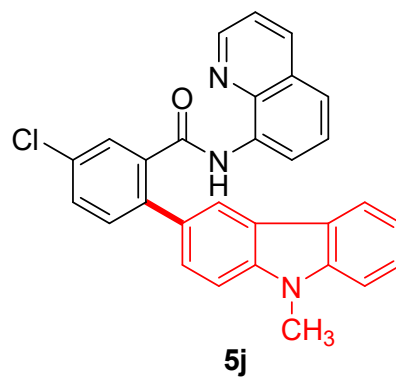
SpinWorks 4: RD 890
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



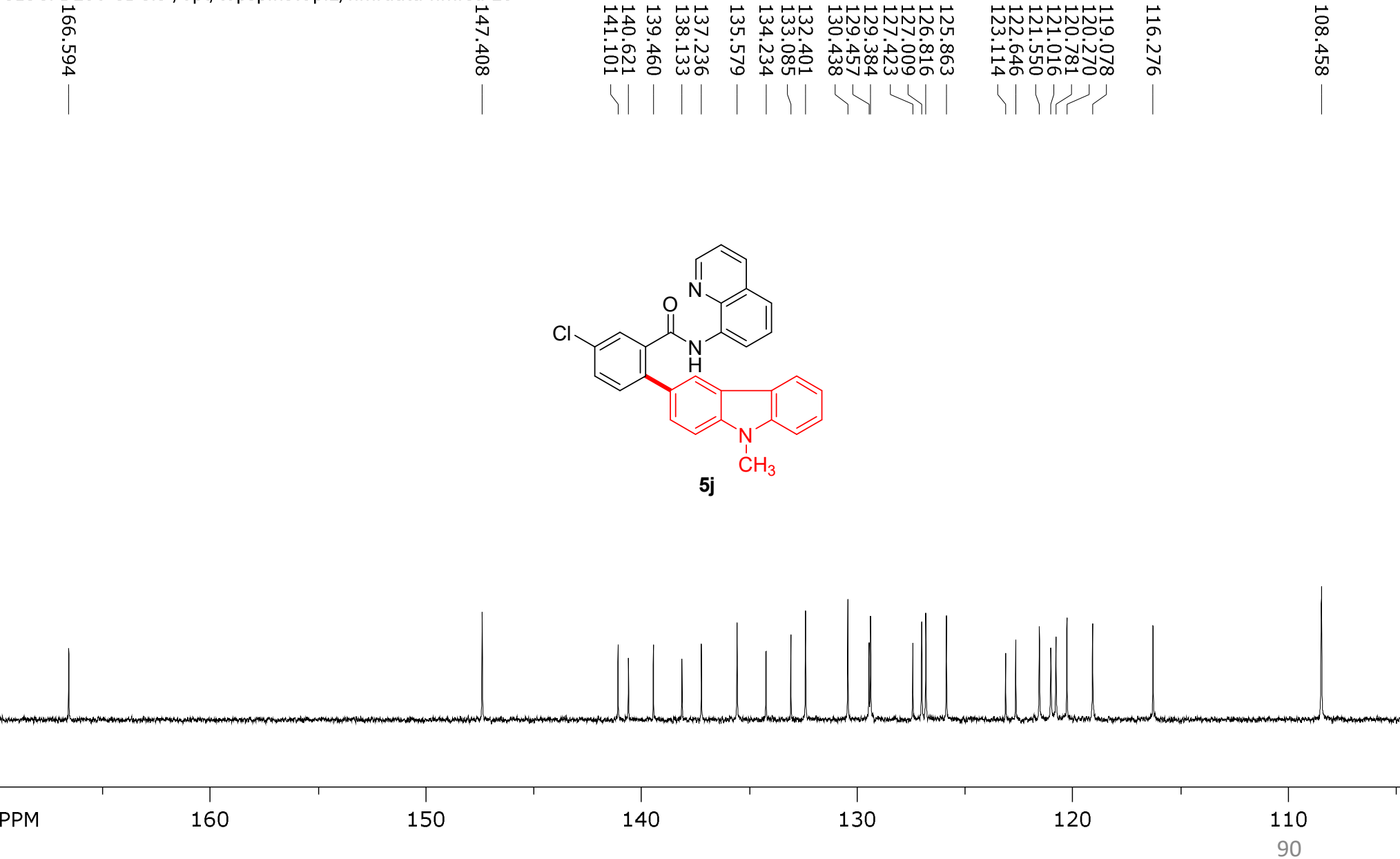
SpinWorks 4: RD 890

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

166.594
147.408
141.101
140.621
139.460
138.133
137.236
135.579
134.234
133.401
133.085
132.401
131.401
125.852
125.852
125.852
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119.078
116.276
108.458
76.702
77.020
77.338
28.871

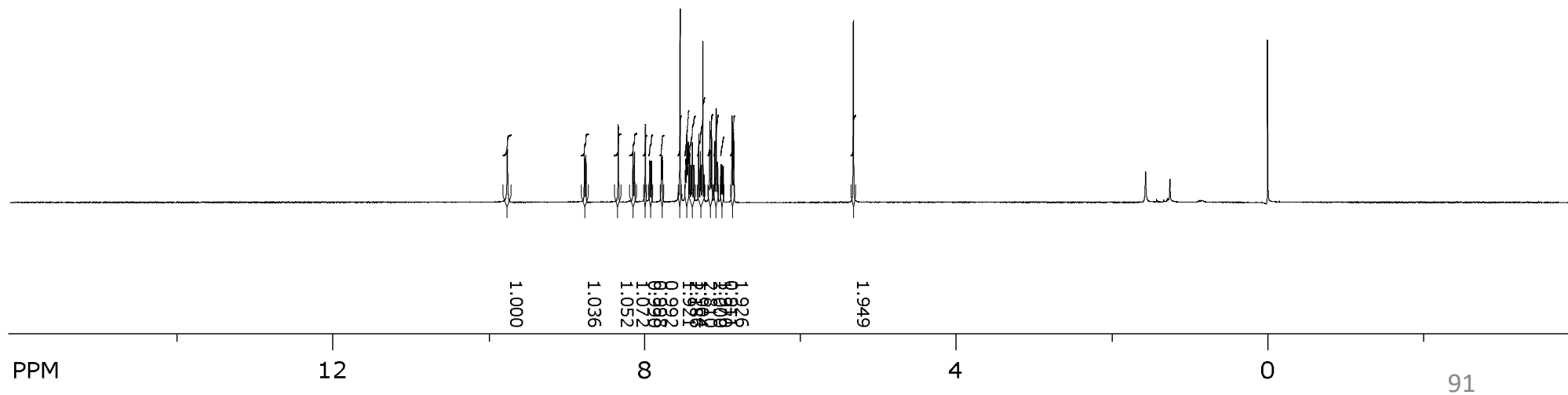
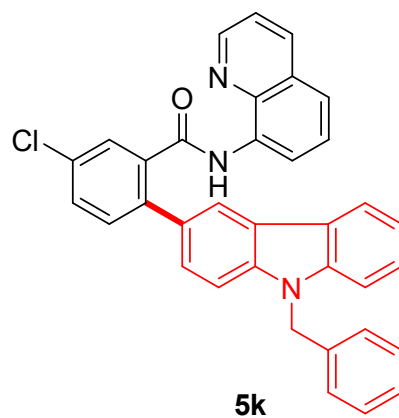


SpinWorks 4: RD 890
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

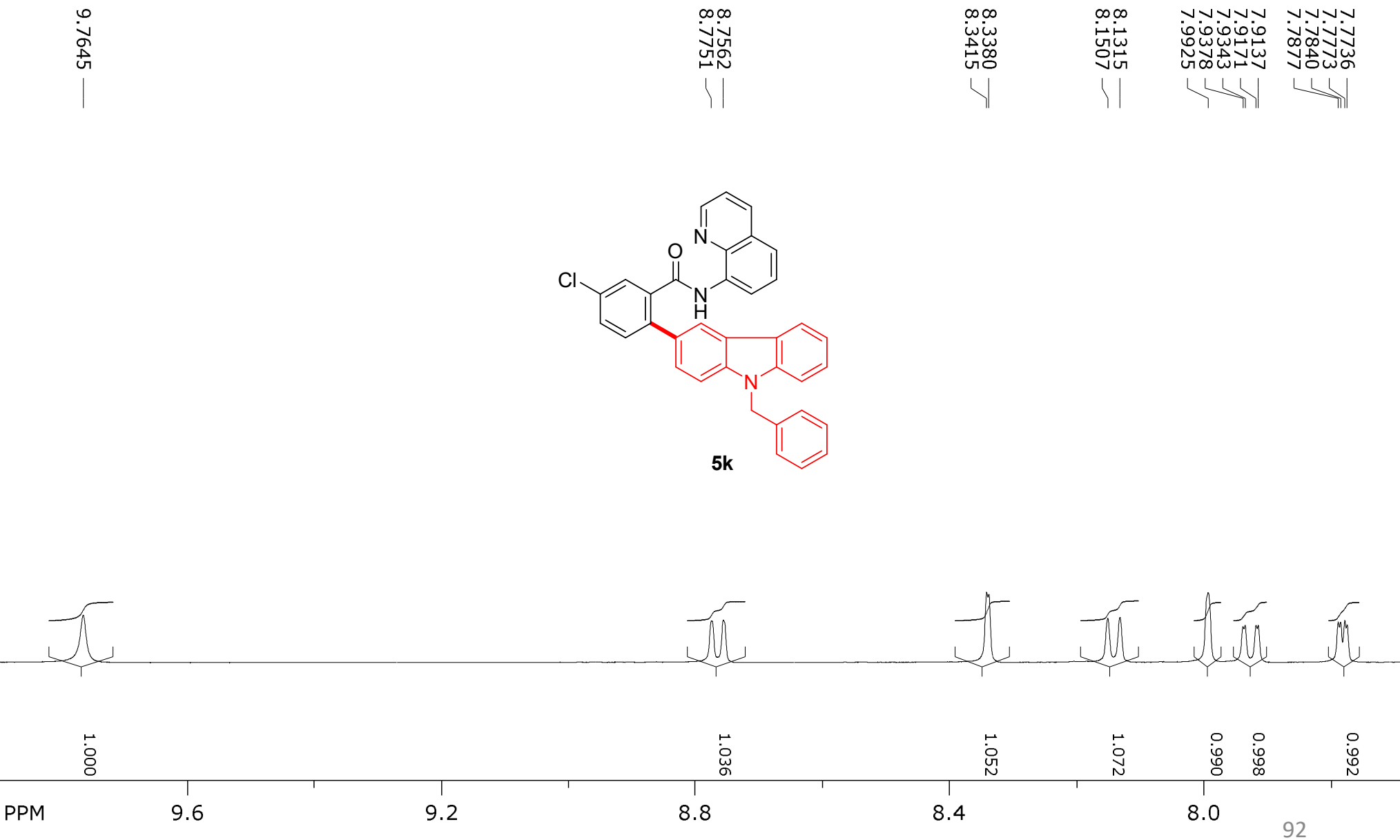


PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 6

5.3206	7.0643	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
6.8587	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
6.8773	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
6.9916	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.0022	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.0122	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.0228	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.0543	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.0916	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.1300	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.1684	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.2068	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.2452	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.2836	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.3220	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.3604	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.3988	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.4372	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.4756	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.5140	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.5524	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.5908	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.6292	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.6676	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.7060	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.7444	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.7828	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.8212	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.8596	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.8980	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.9364	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
7.9748	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
8.0132	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
8.0516	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
8.0900	7.0916	7.7839	7.9925	8.1315	8.3415	8.7562	8.7751	9.7645
8.1284	7.0916	7.7839	7.9925	8.1315				

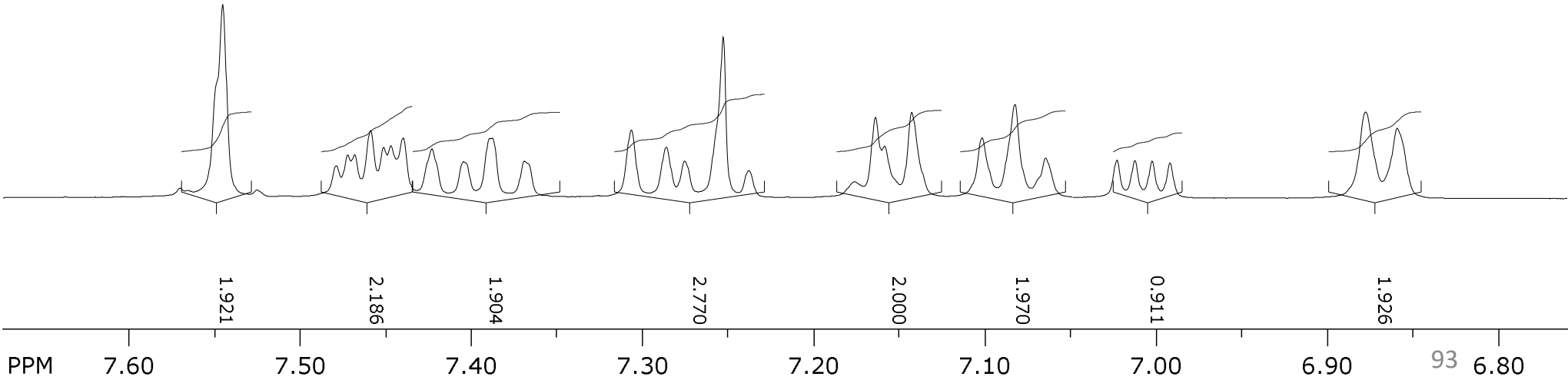
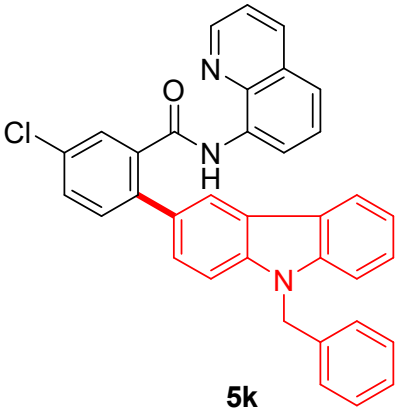


SpinWorks 4: RD-892
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 6

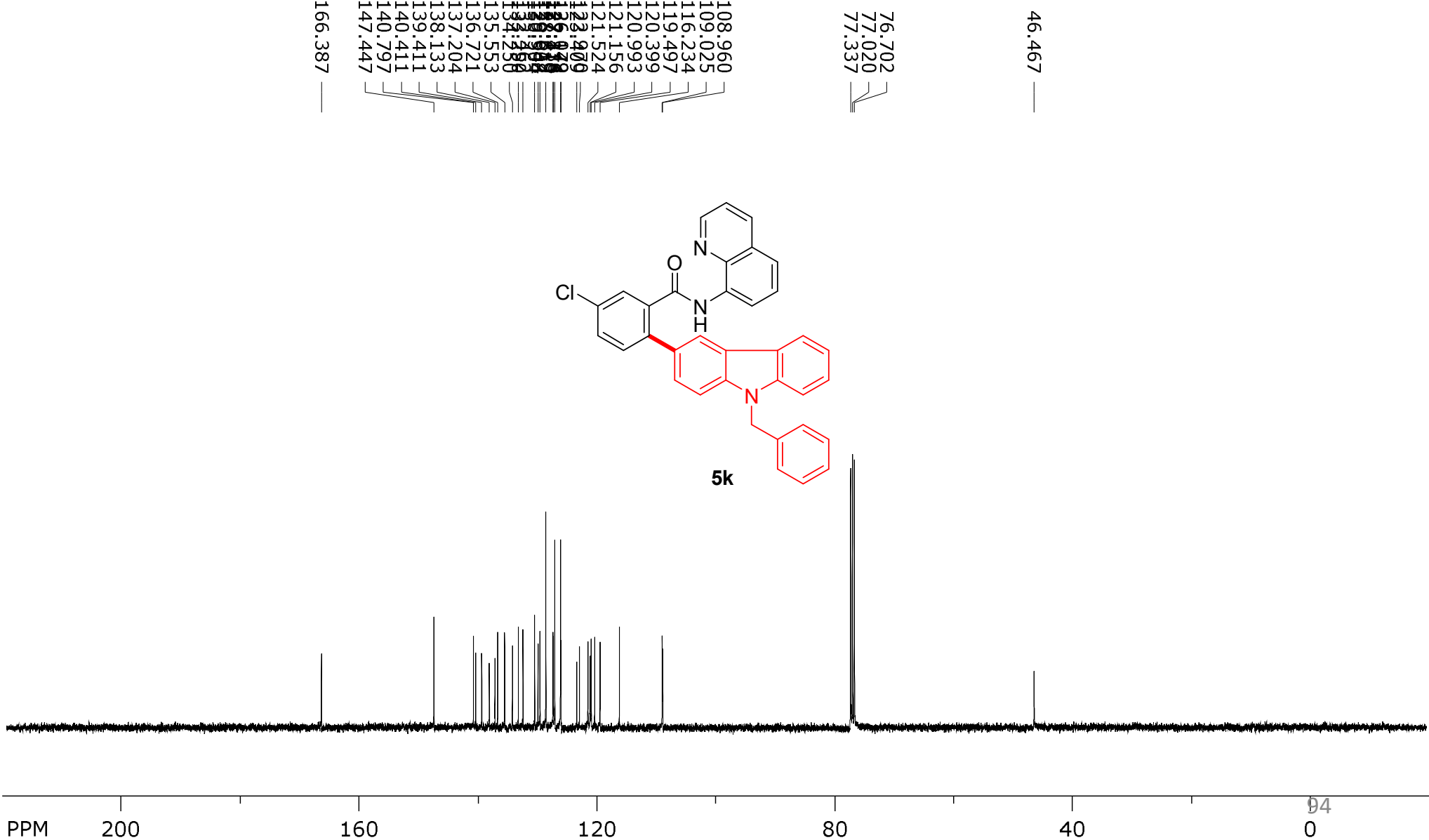


SpinWorks 4: RD-892
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 6

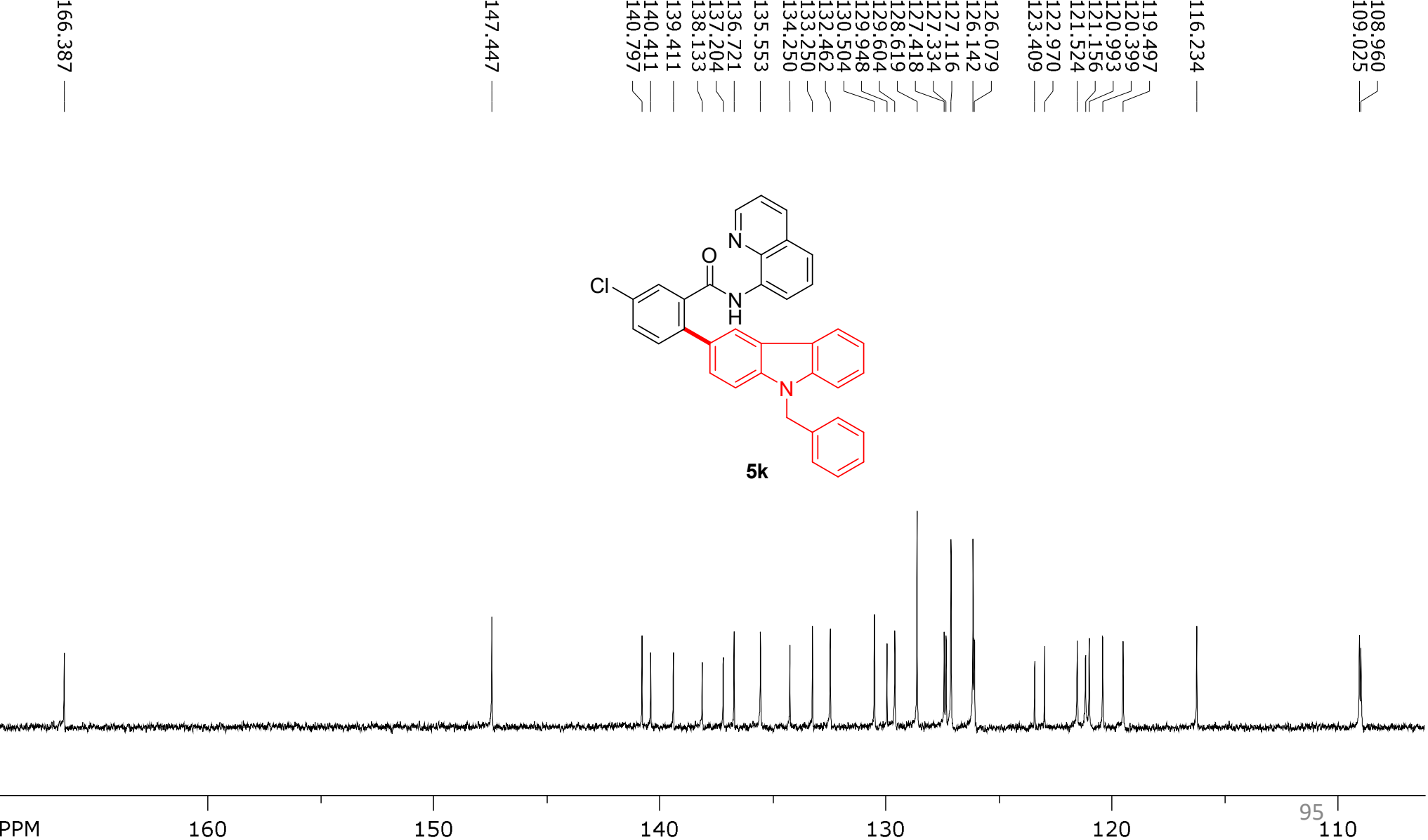
7.5456	7.3692	7.2381	7.1426	7.0643	6.9916	6.8587
—	7.3878	7.2530	7.1586	—	7.0022	—
	7.3895	—	7.1639	7.0824	7.0122	
	7.4049	7.3067	7.1756	7.1017	7.0228	6.8773
	7.4233	—	—	—	—	—
	7.4402	—	—	—	—	—
	7.4472	—	—	—	—	—
	7.4514	—	—	—	—	—
	7.4592	—	—	—	—	—
	7.4685	—	—	—	—	—
	7.4725	—	—	—	—	—
	7.4792	—	—	—	—	—

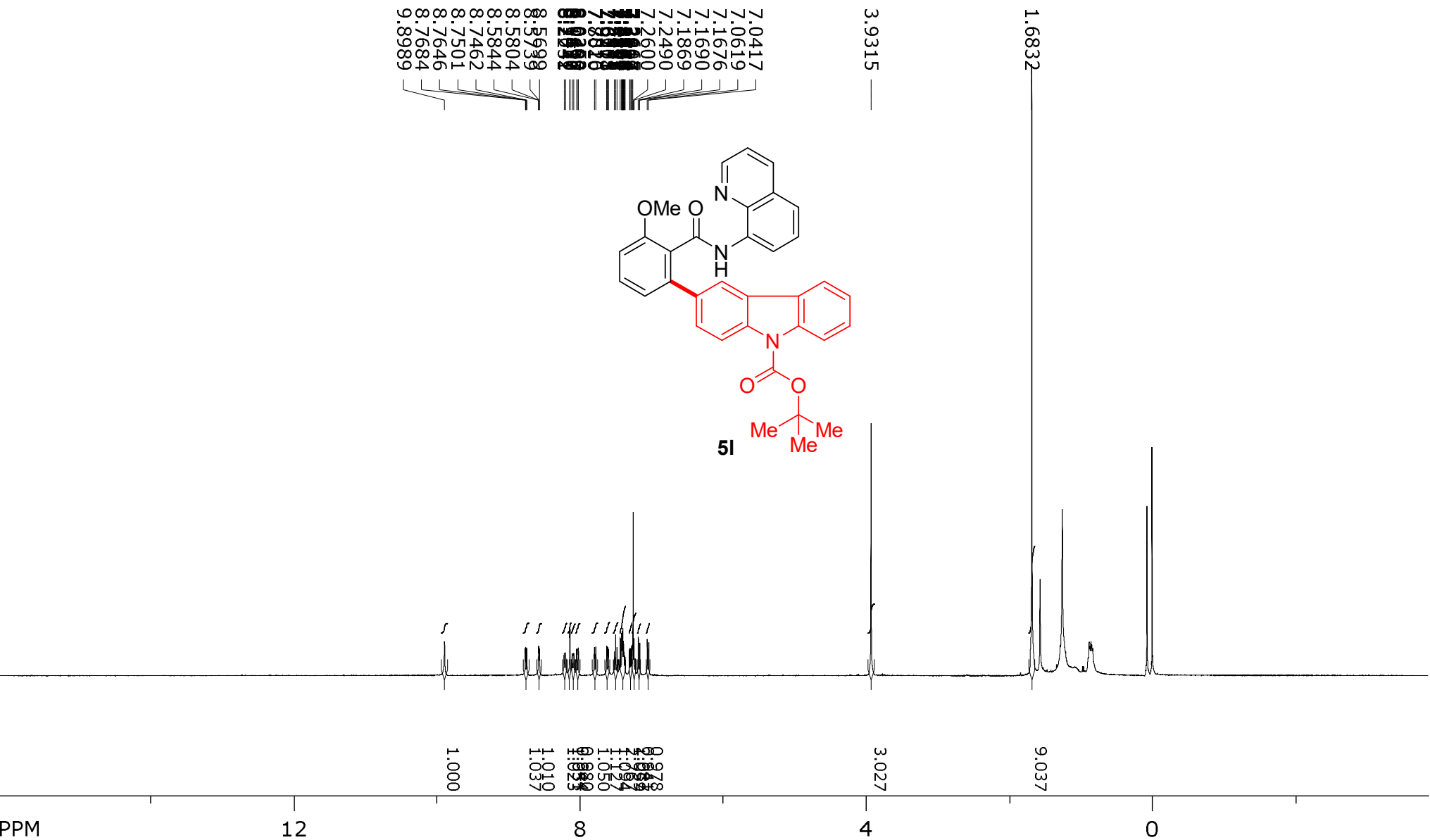


SpinWorks 4: RD-892
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

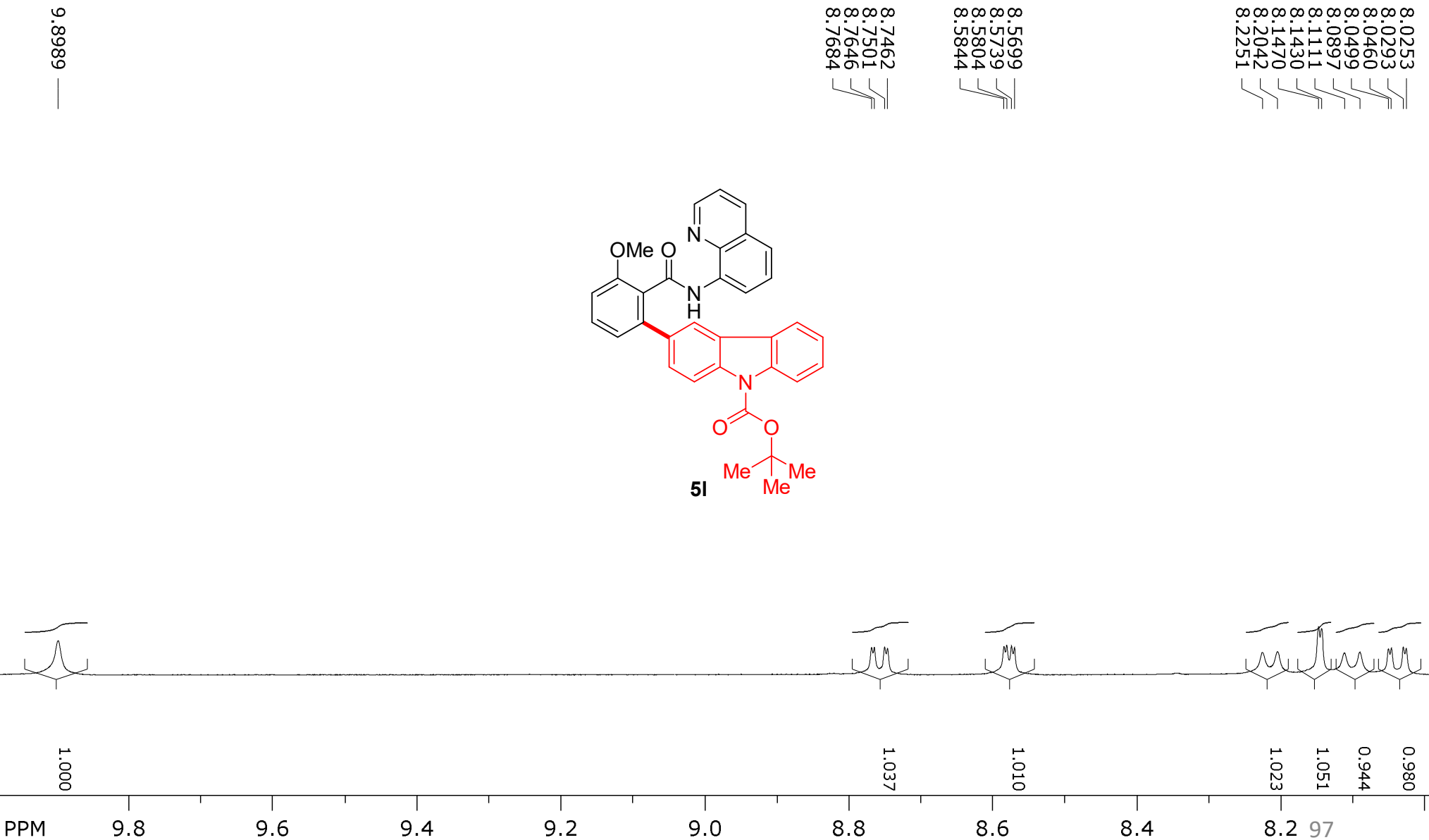


SpinWorks 4: RD-892
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

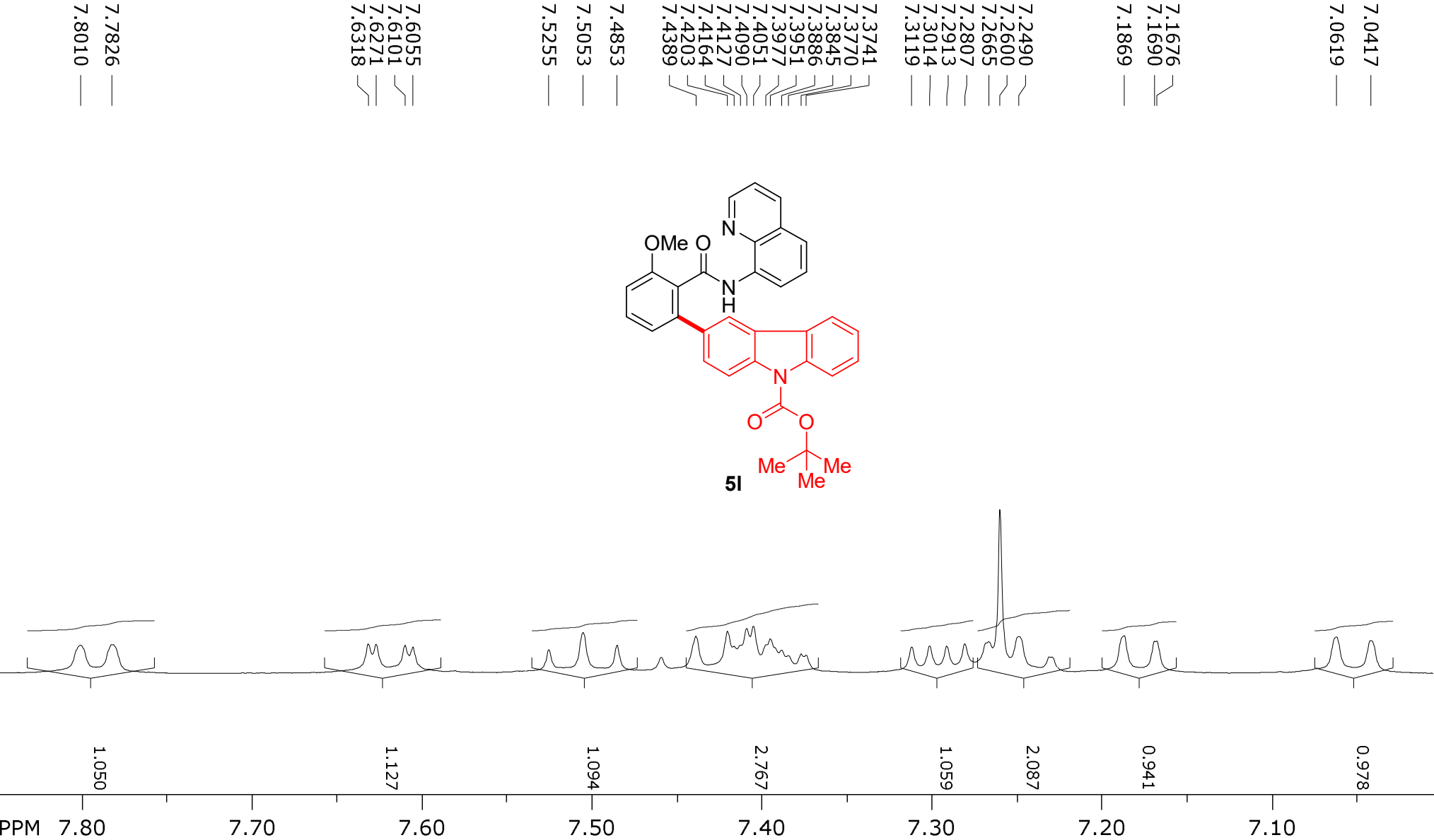




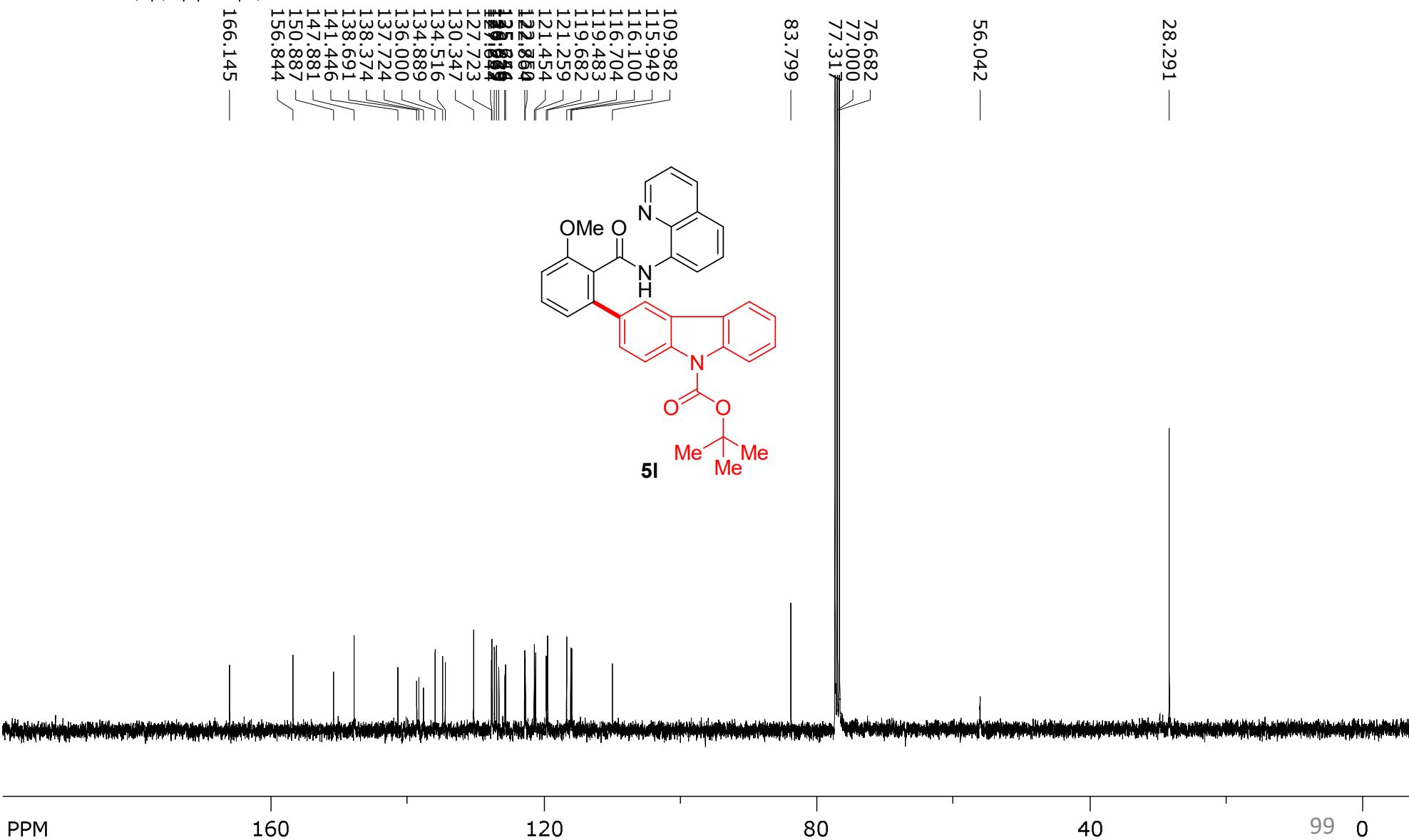
SpinWorks 4: RD 740



SpinWorks 4: RD 740

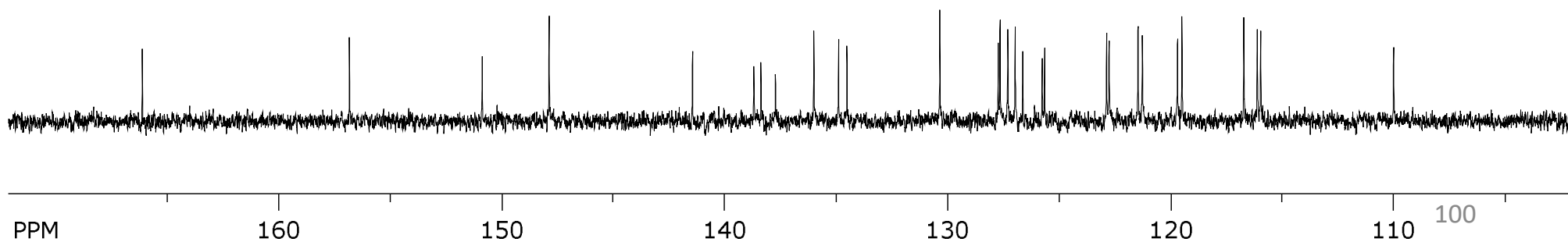
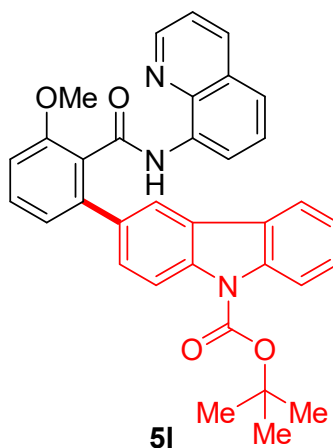


SpinWorks 4: RD-740
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30

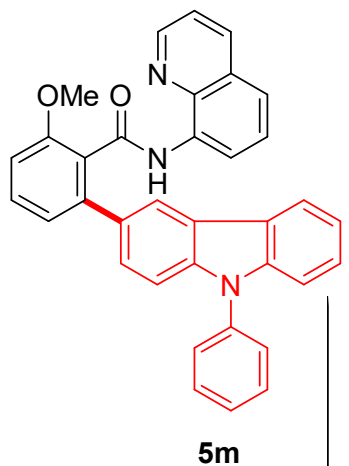


SpinWorks 4: RD-740
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30

166.145	156.844	150.887	147.881	141.446	138.691	137.724	136.000	134.889	134.516	130.347	127.723	127.644	127.297	126.969	126.629	125.756	125.644	122.864	121.454	121.259	119.682	119.483	116.704	116.100	115.949	109.982
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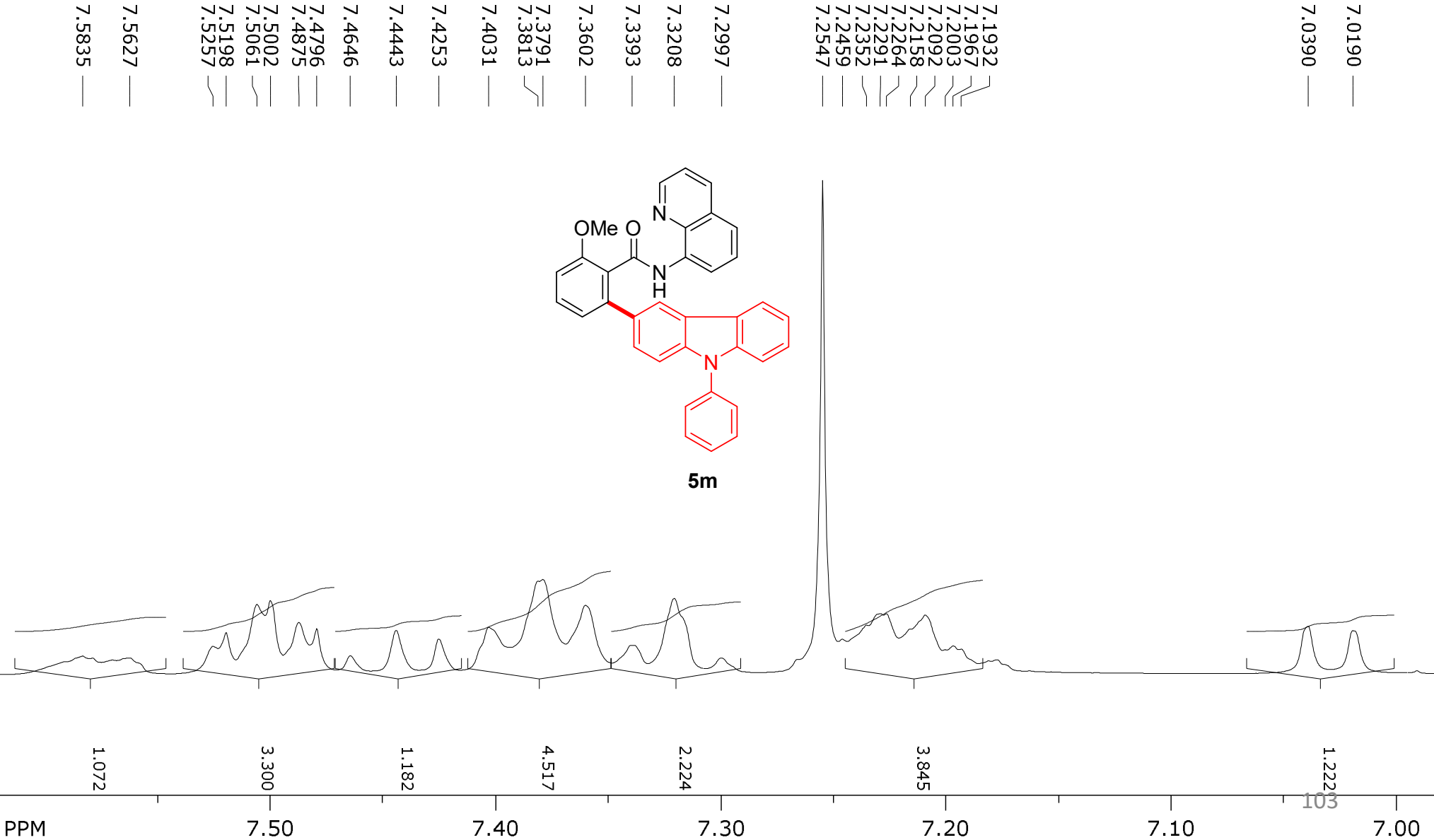
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



SpinWorks 4: RD-1286
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



SpinWorks 4: RD-1286
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

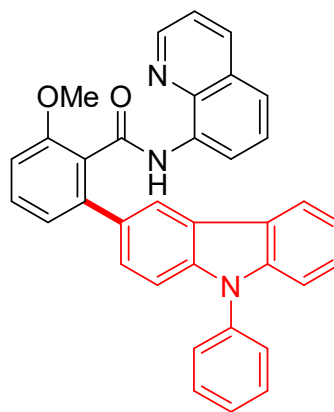


C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 35

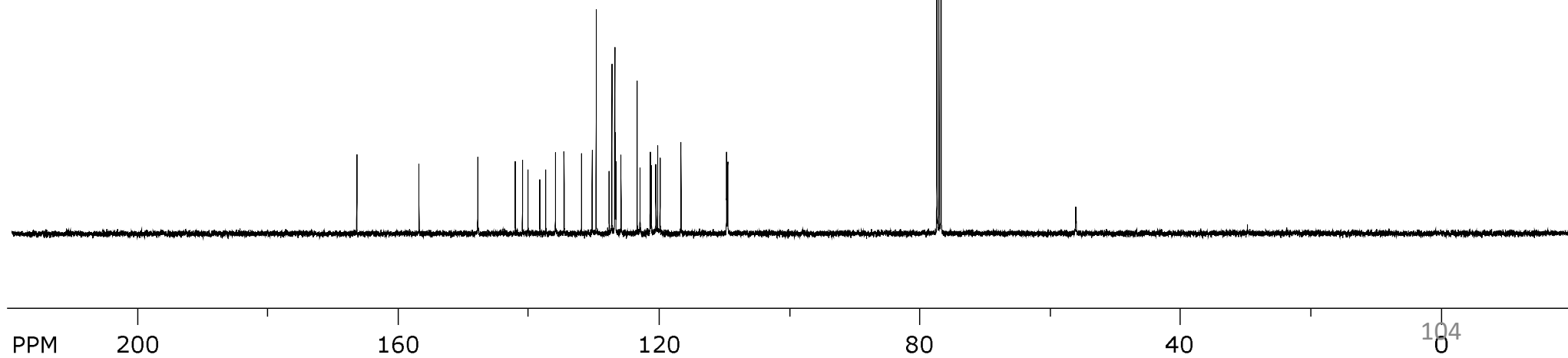
[illegible]

76.702
77.020
77.337

55.989



5m



SpinWorks 4: RD-1286
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 35

166.390 —

156.835 —

147.812 —

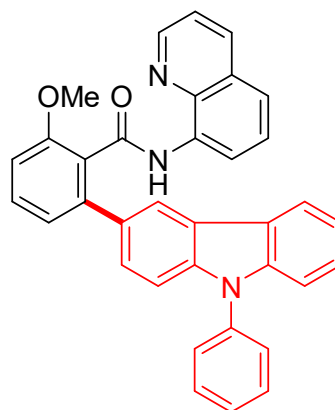
142.067 —
140.961 —
140.108 —

138.293 —
137.383 —
135.892 —
134.571 —

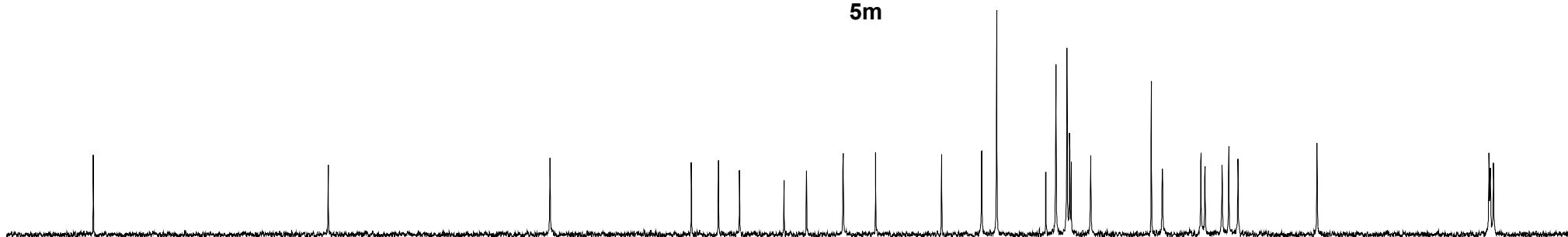
131.888 —
130.259 —
129.649 —
127.649 —
127.238 —
126.790 —
126.681 —
126.618 —
125.824 —

123.359 —
122.908 —
121.340 —
120.480 —
120.208 —
119.831 —
116.619 —

109.625 —
109.572 —
109.441 —



5m



PPM

160

150

140

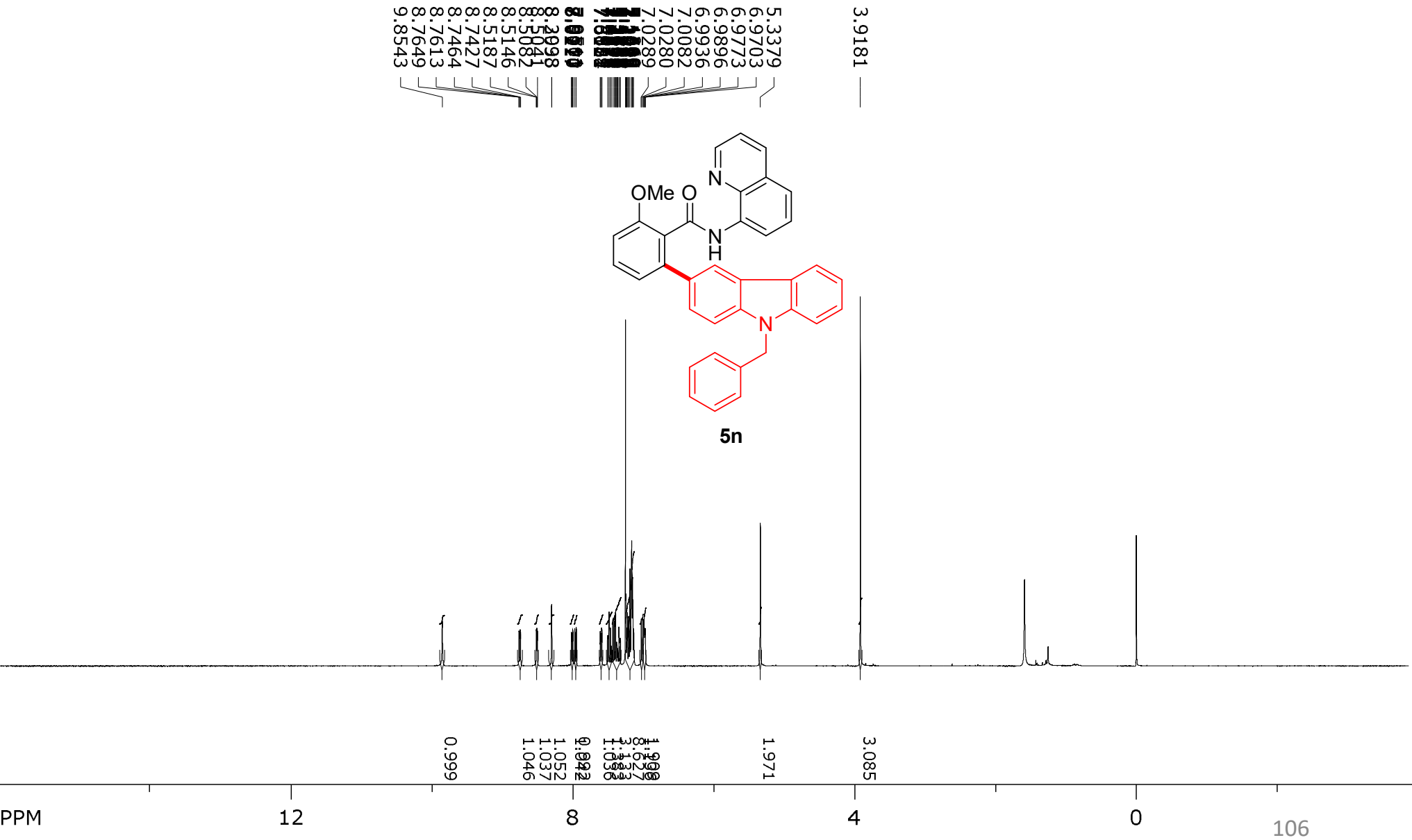
130

120

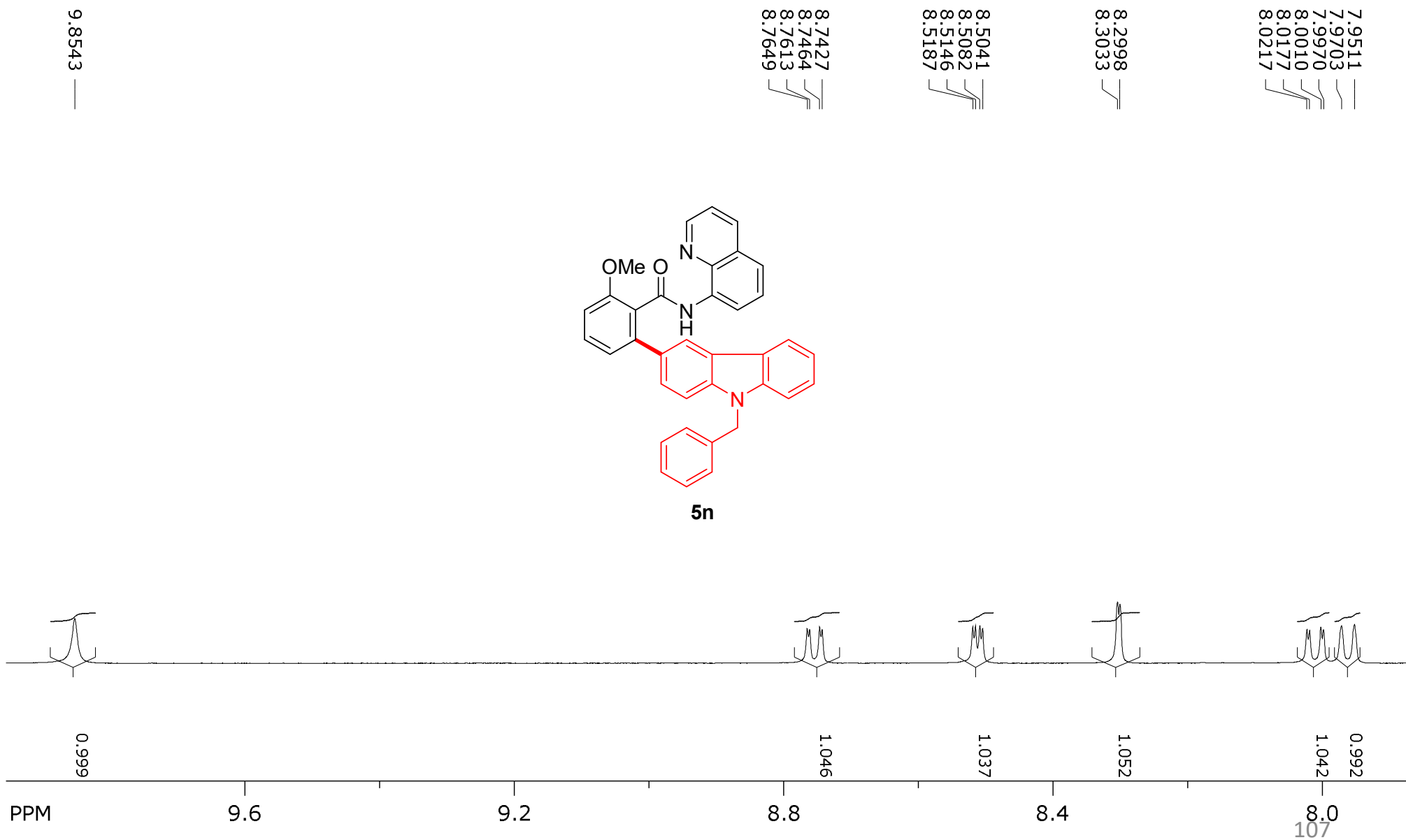
110

105

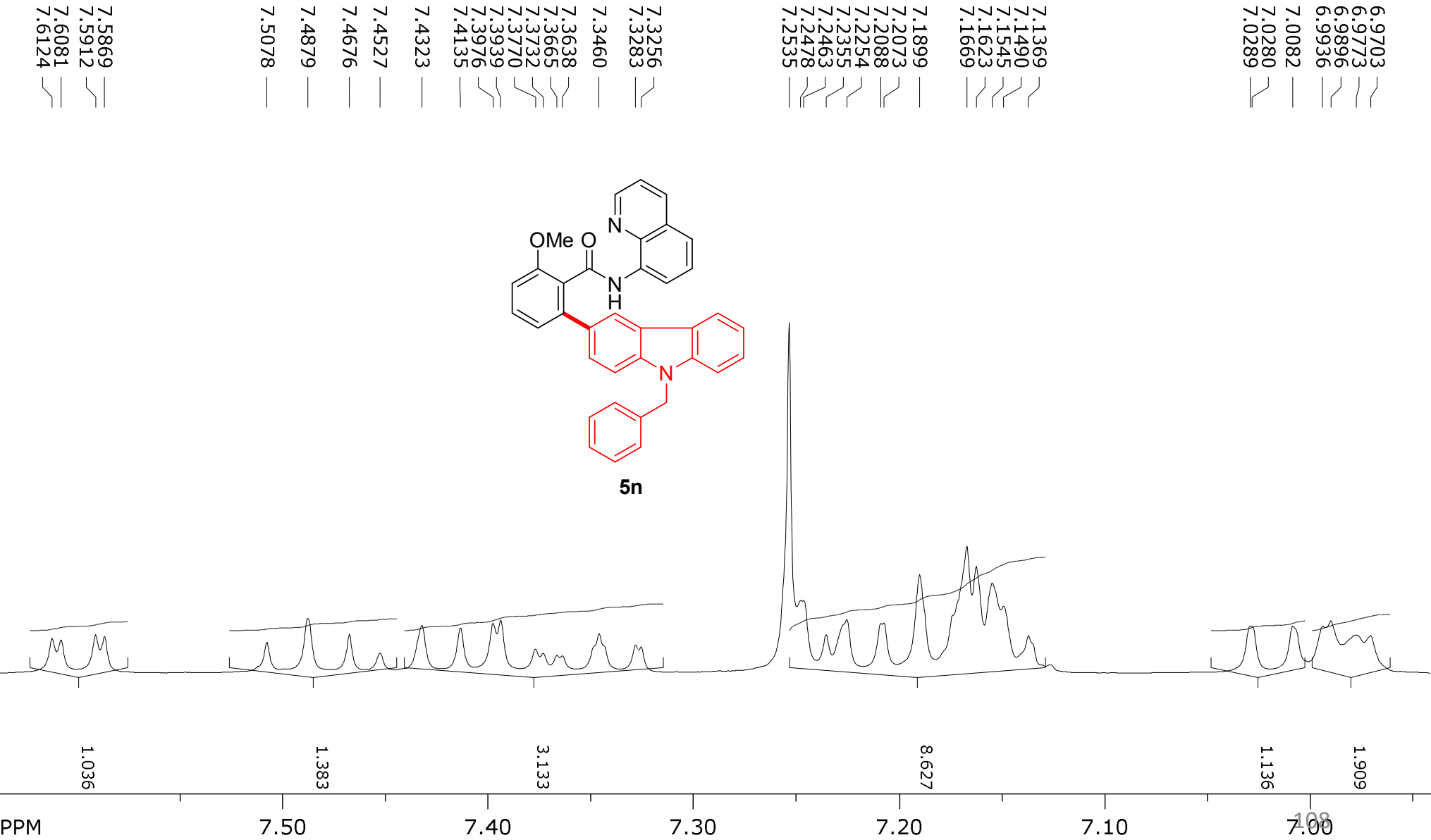
SpinWorks 4: RD-1280
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



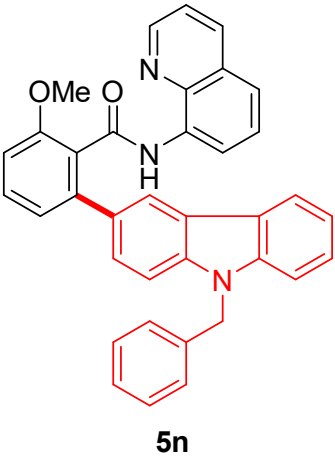
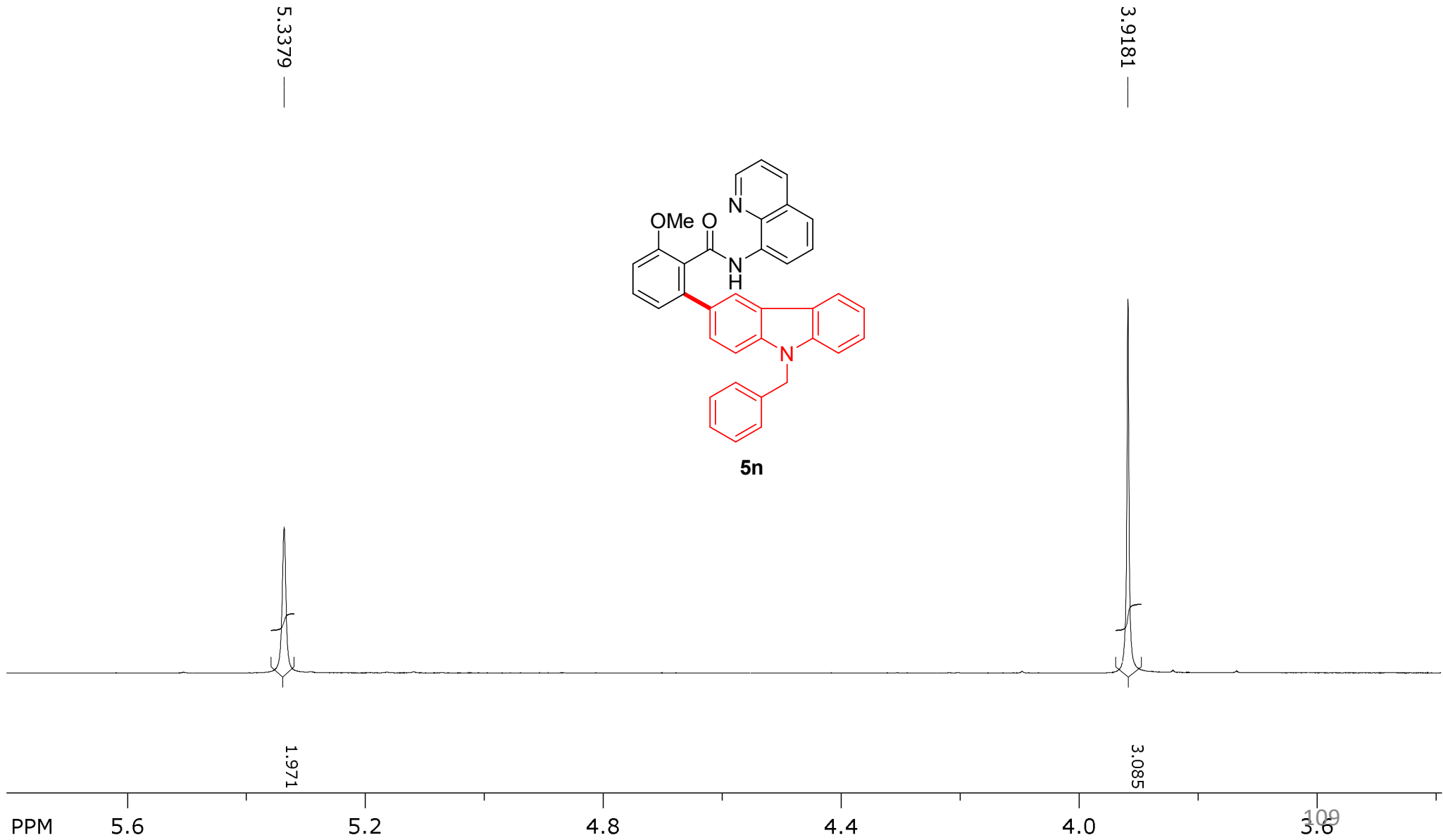
SpinWorks 4: RD-1280
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



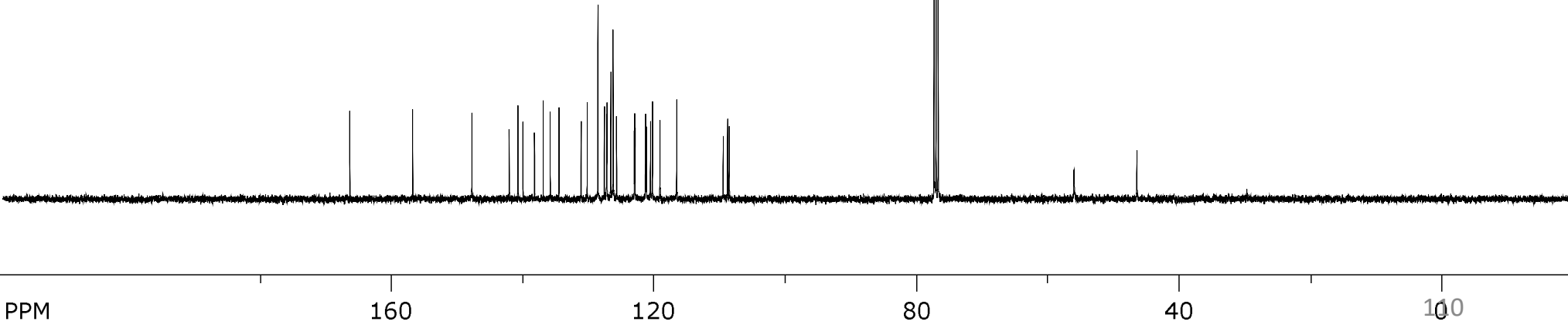
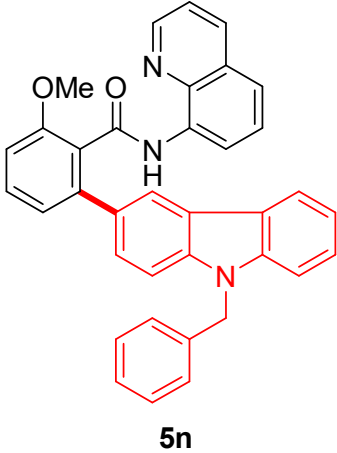
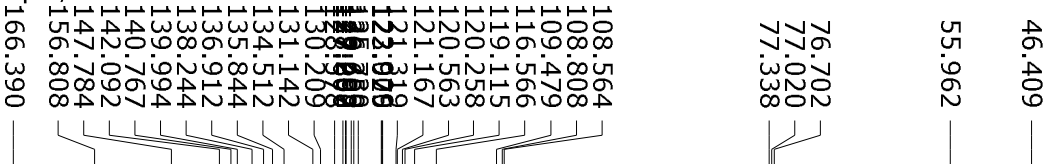
SpinWorks 4: RD-1280
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



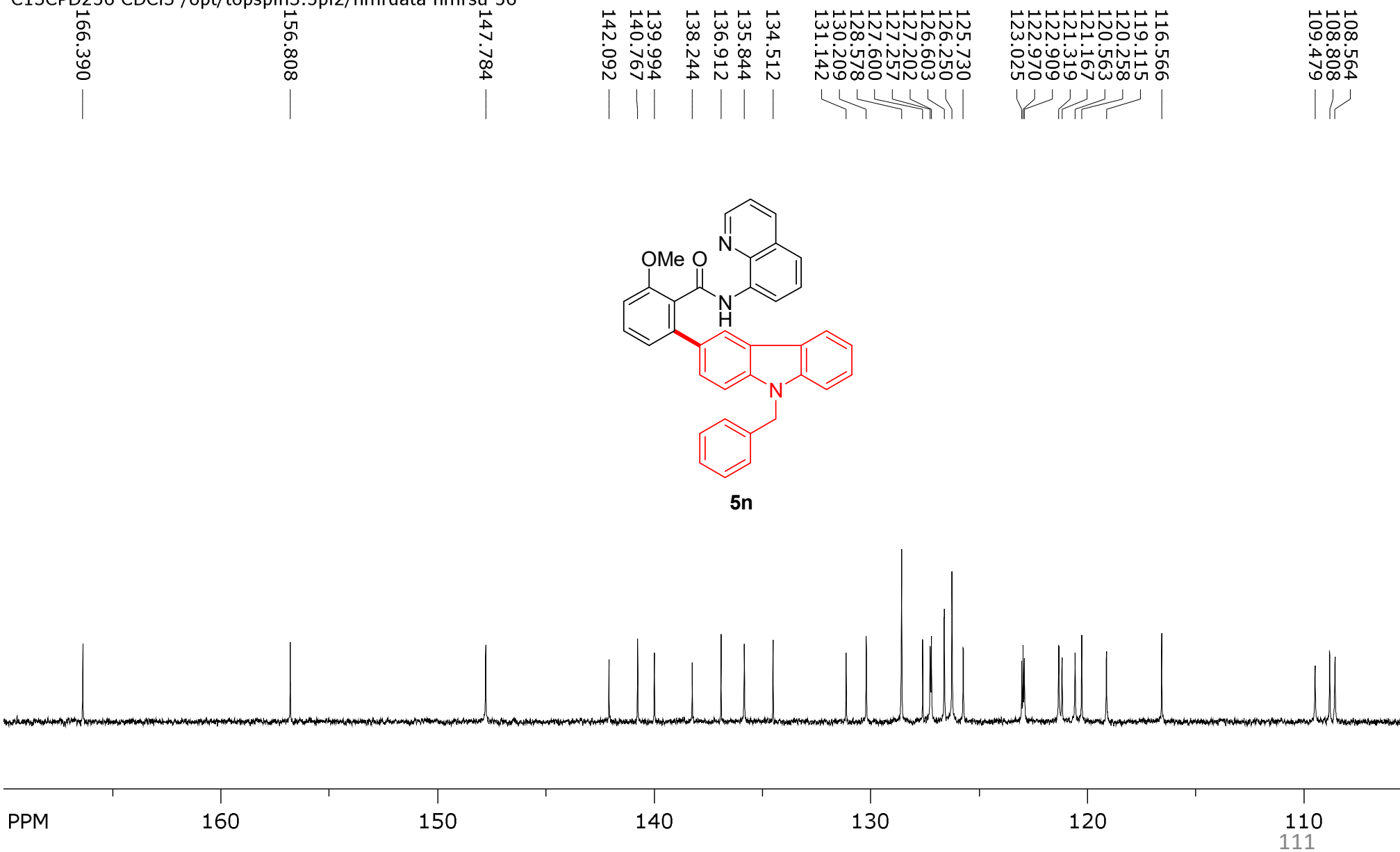
SpinWorks 4: RD-1280
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



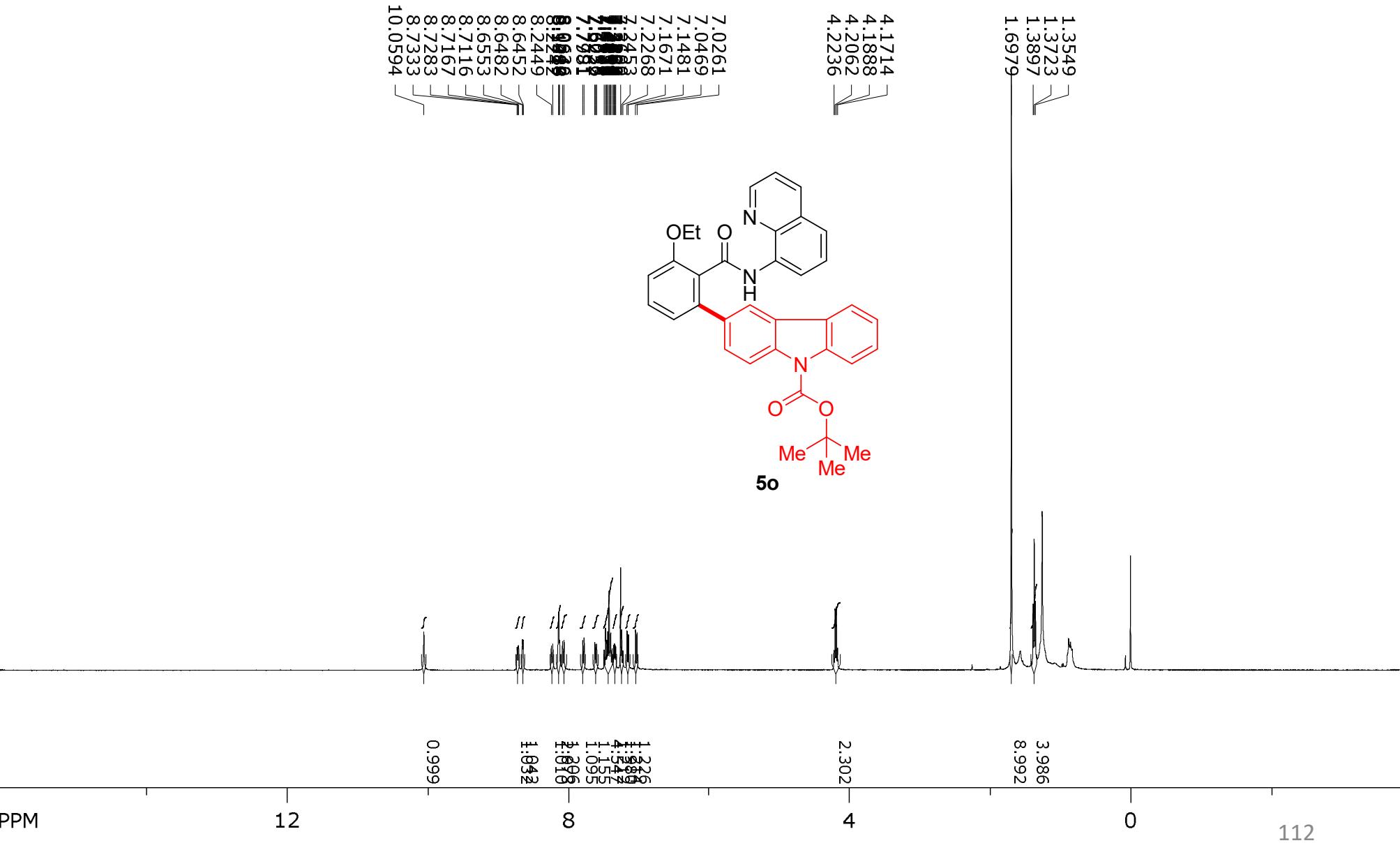
SpinWorks 4: RD-1280
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56



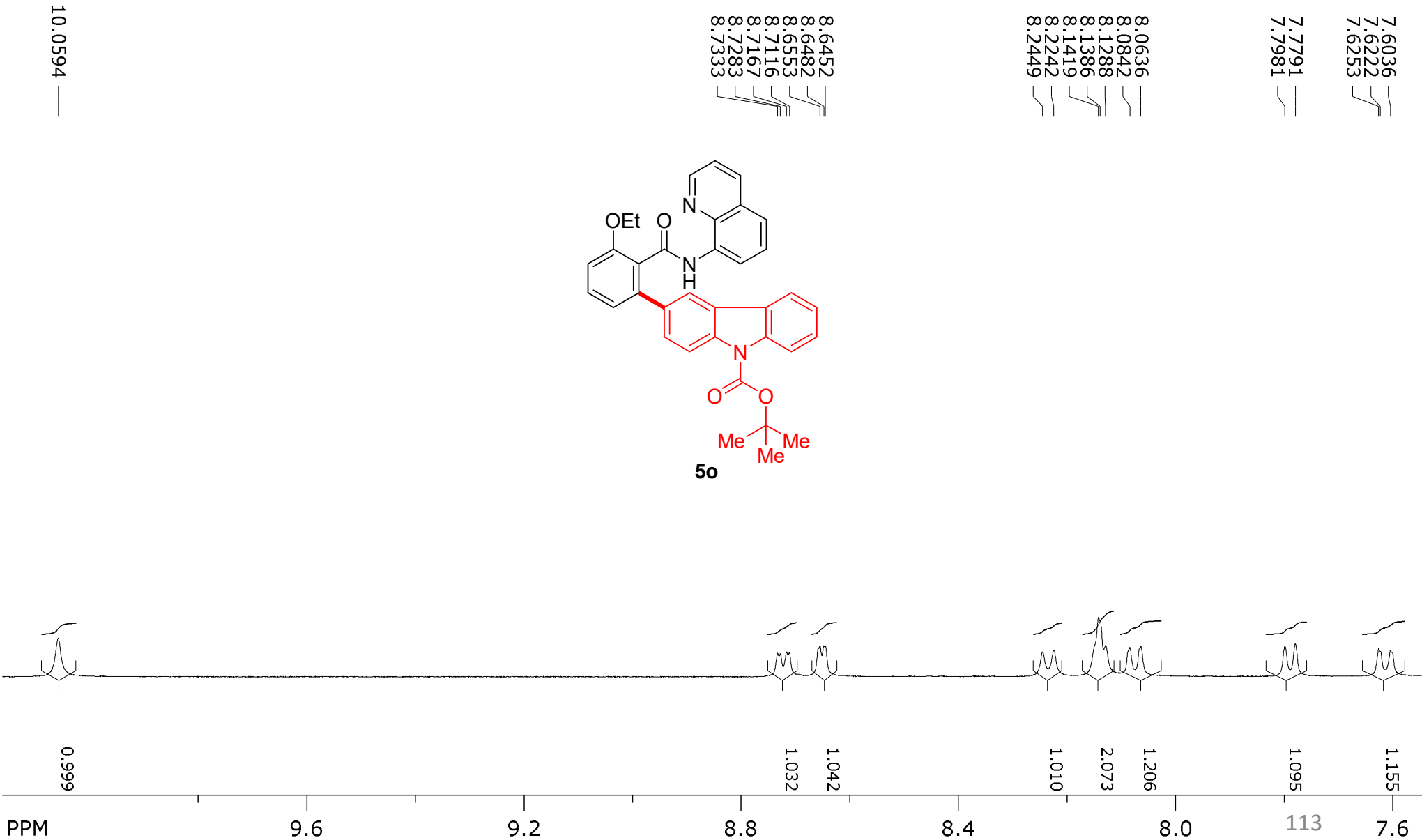
SpinWorks 4: RD-1280
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56



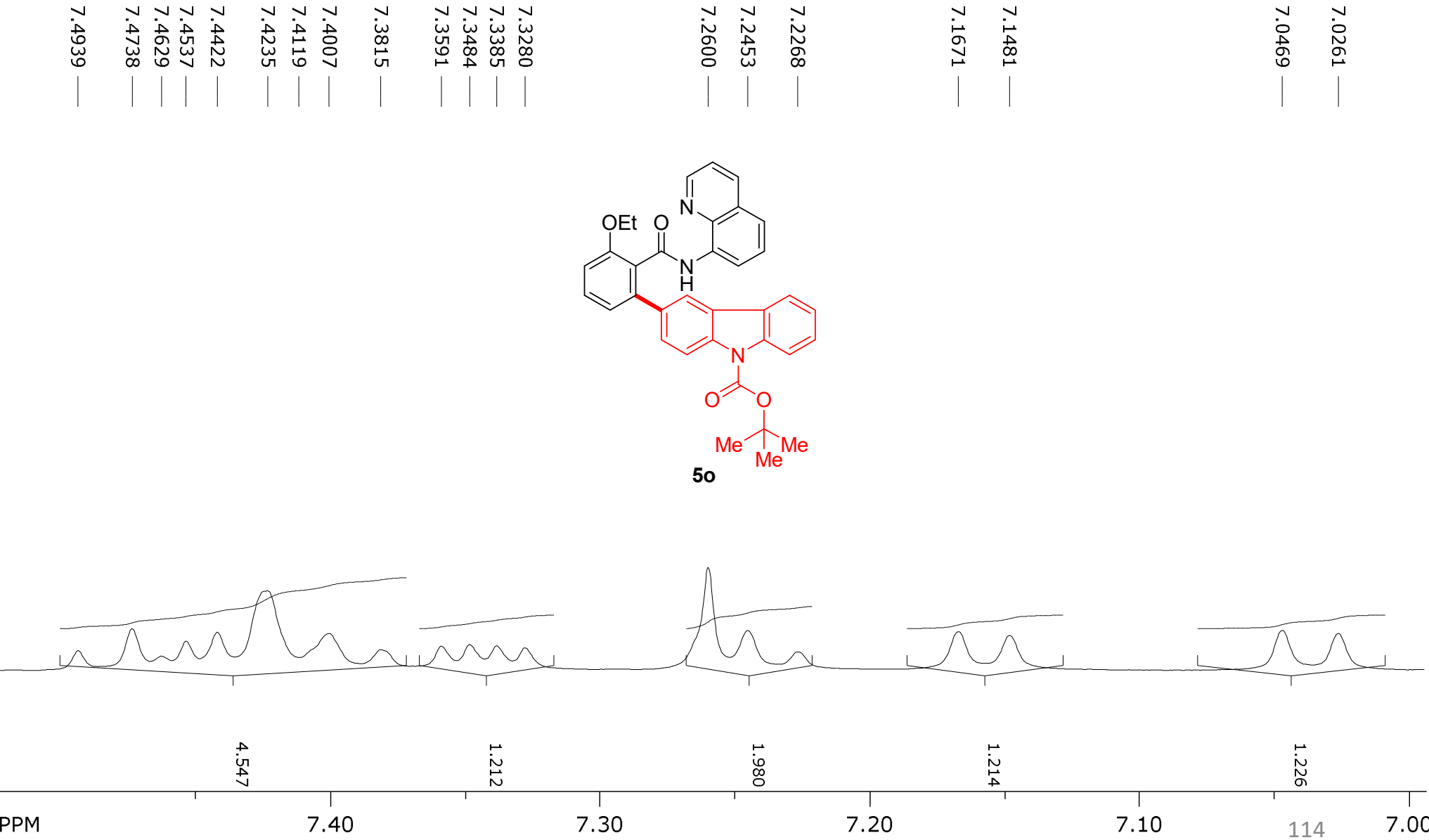
SpinWorks 4: rd 722

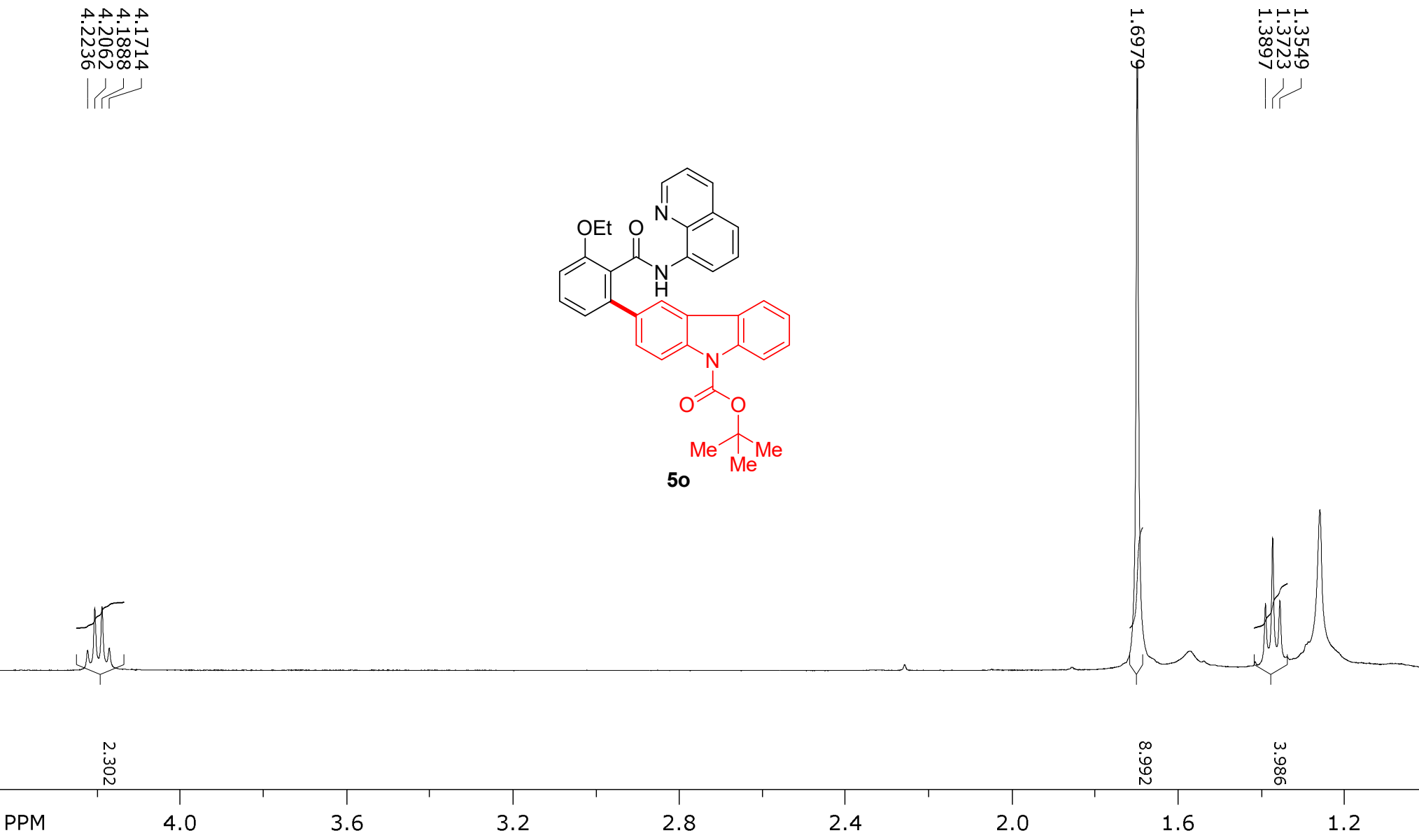


SpinWorks 4: rd 722

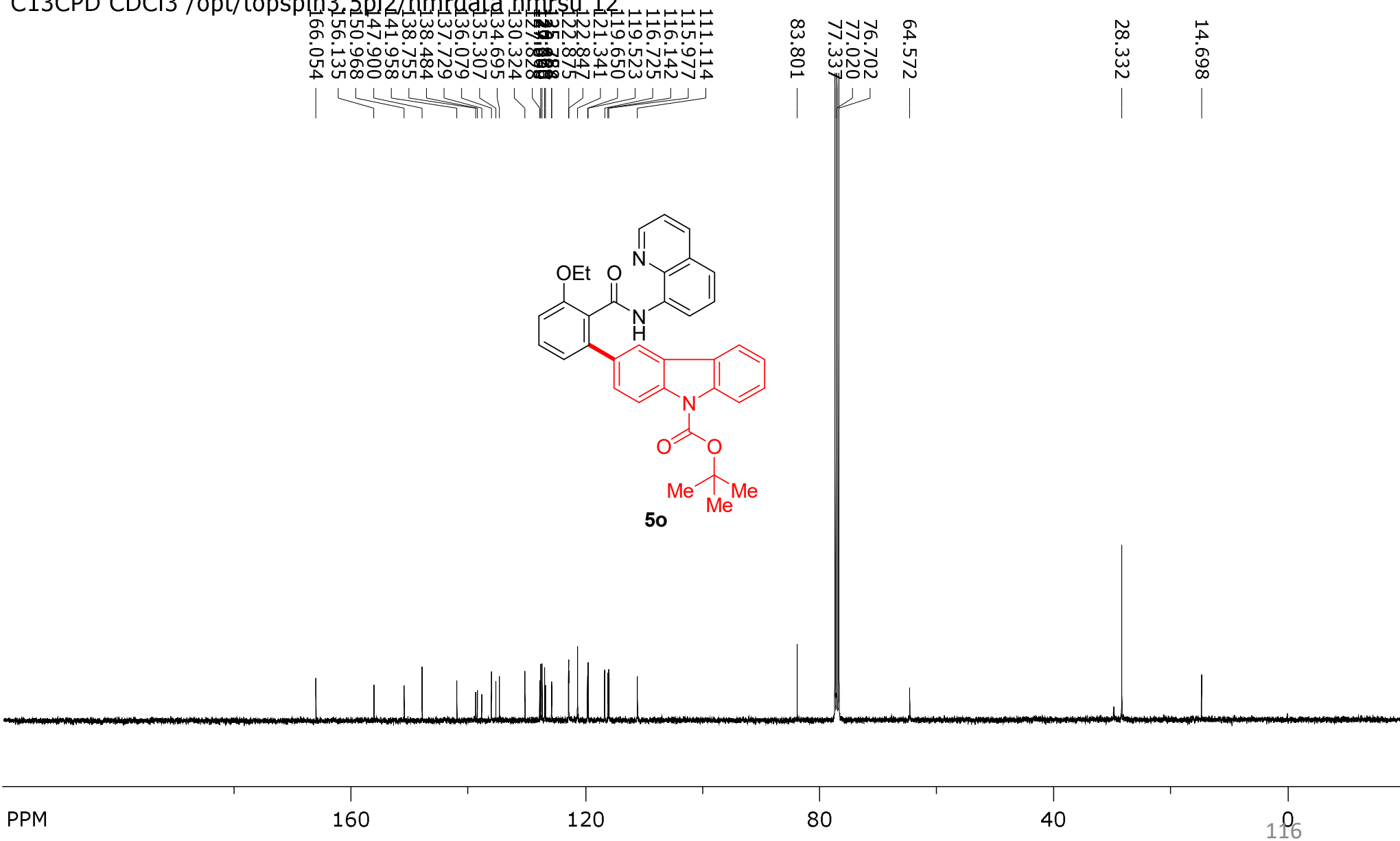


SpinWorks 4: rd 722

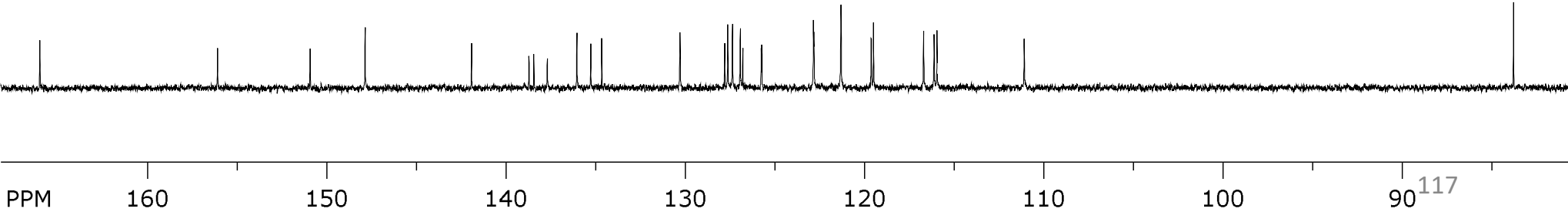
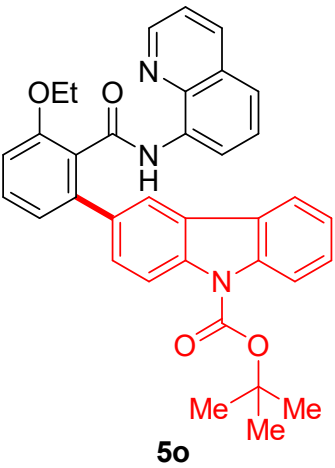
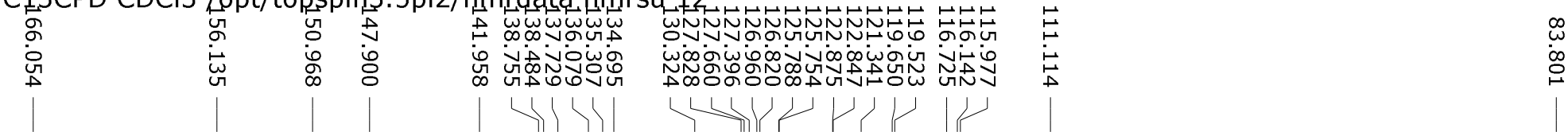


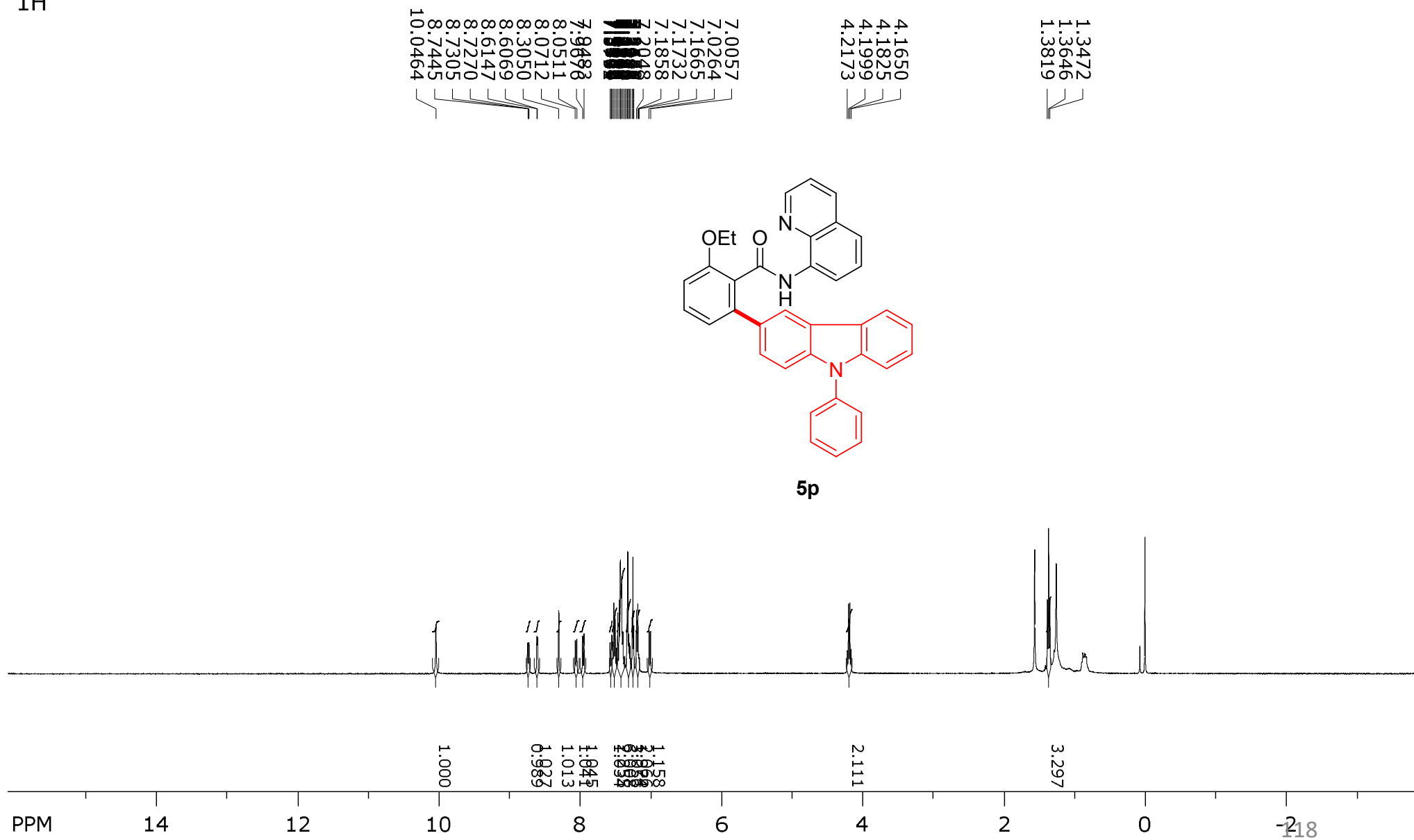


SpinWorks 4: RD 722
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

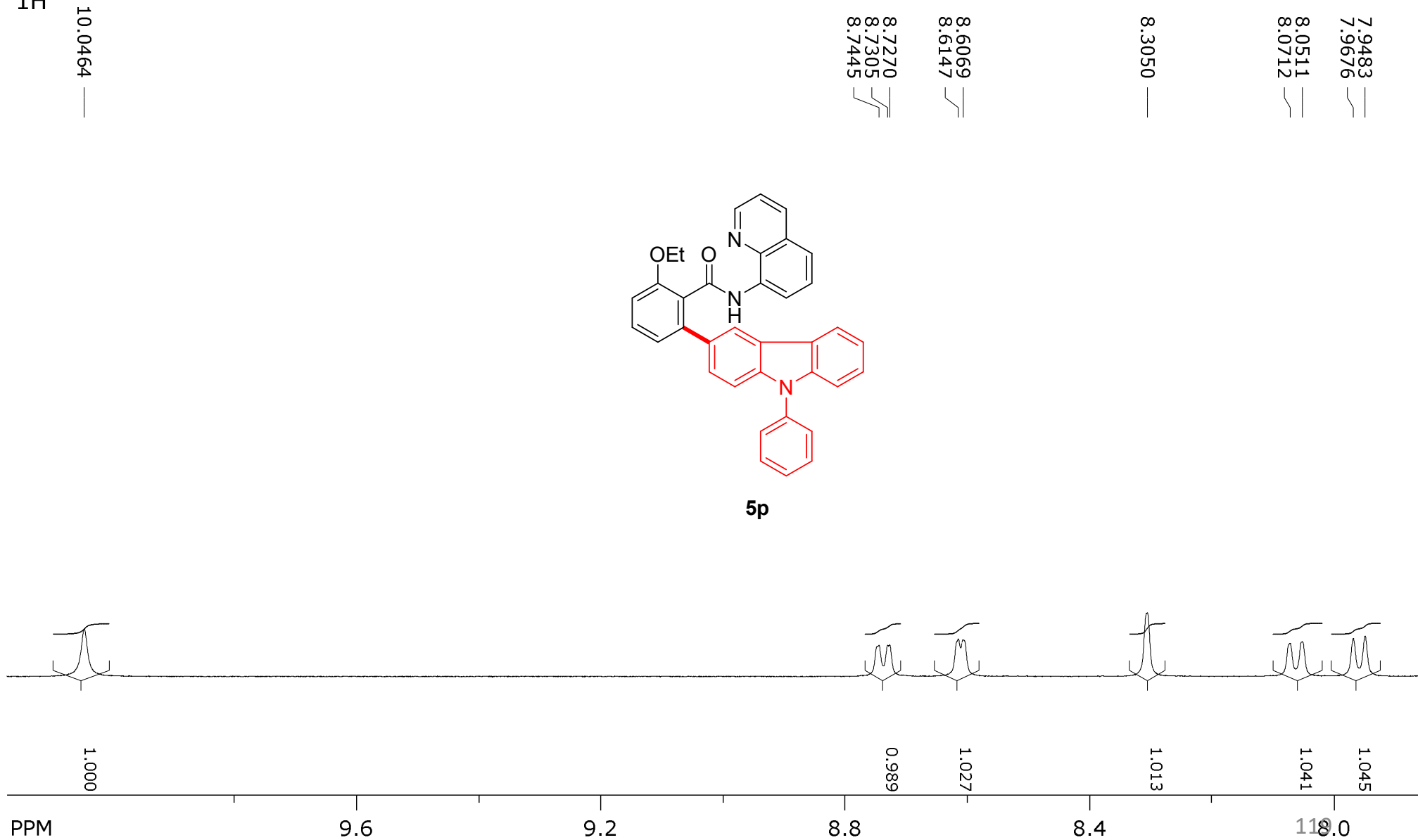


SpinWorks 4: RD 722
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu_12



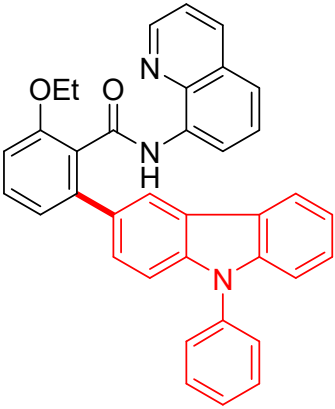
SpinWorks 4: RD 721
1H

SpinWorks 4: RD 721
1H

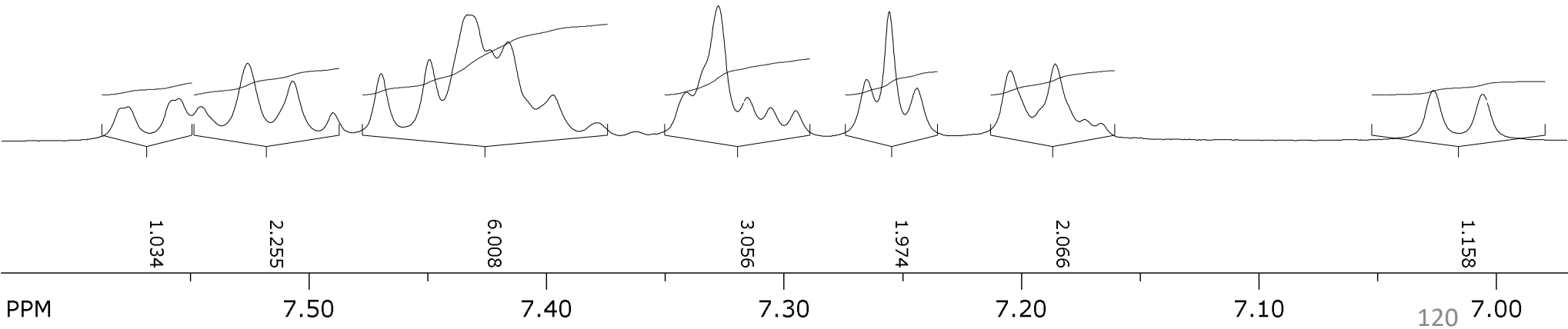


SpinWorks 4: RD 721
1H

7.0057 —
7.0264 —
7.1665 —
7.1732 —
7.1858 —
7.2048 —
7.2440 —
7.2557 —
7.2651 —
7.2951 —
7.3056 —
7.3155 —
7.3276 —
7.3410 —
7.3619 —
7.3633 —
7.3784 —
7.3790 —
7.3973 —
7.4162 —
7.4240 —
7.4319 —
7.4330 —
7.4493 —
7.4697 —
7.4899 —
7.5069 —
7.5258 —
7.5456 —
7.5549 —
7.5574 —
7.5762 —
7.5791 —



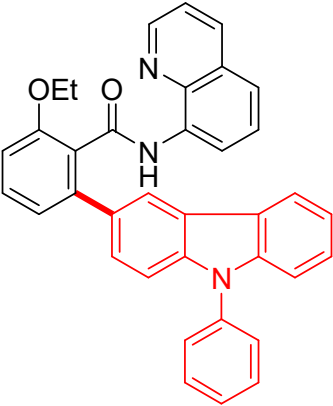
5p



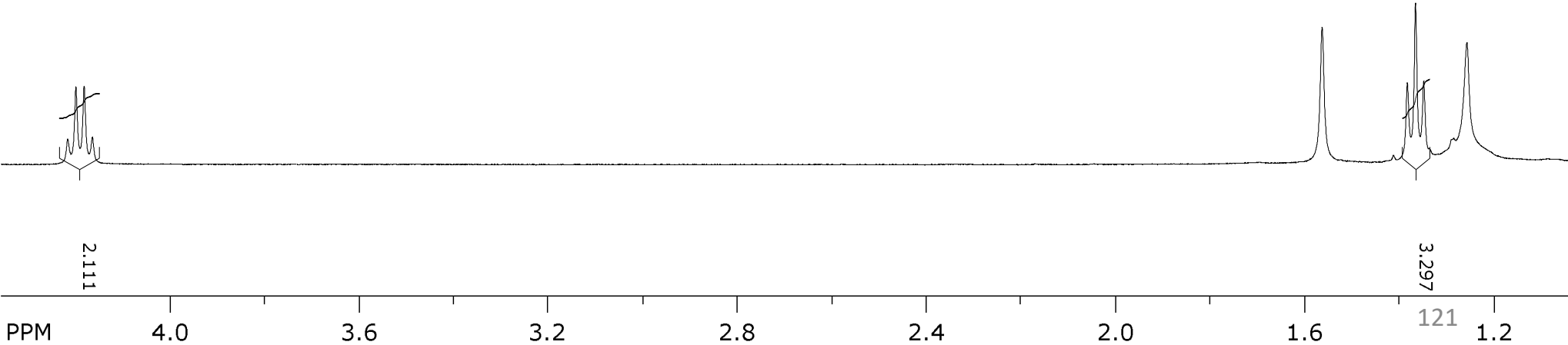
SpinWorks 4: RD 721
1H

4.1650
4.1825
4.1999
4.2173

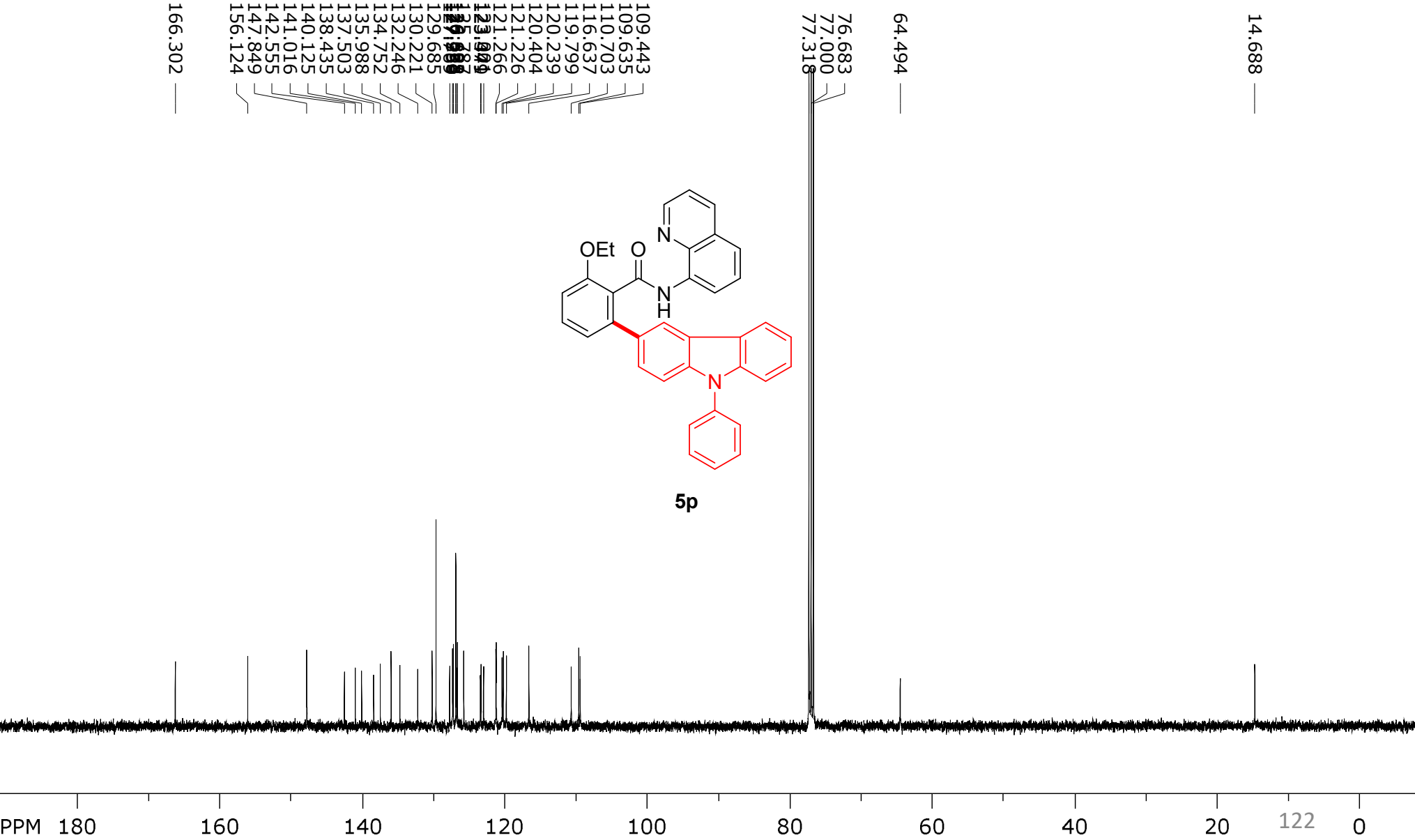
1.3472
1.3646
1.3819



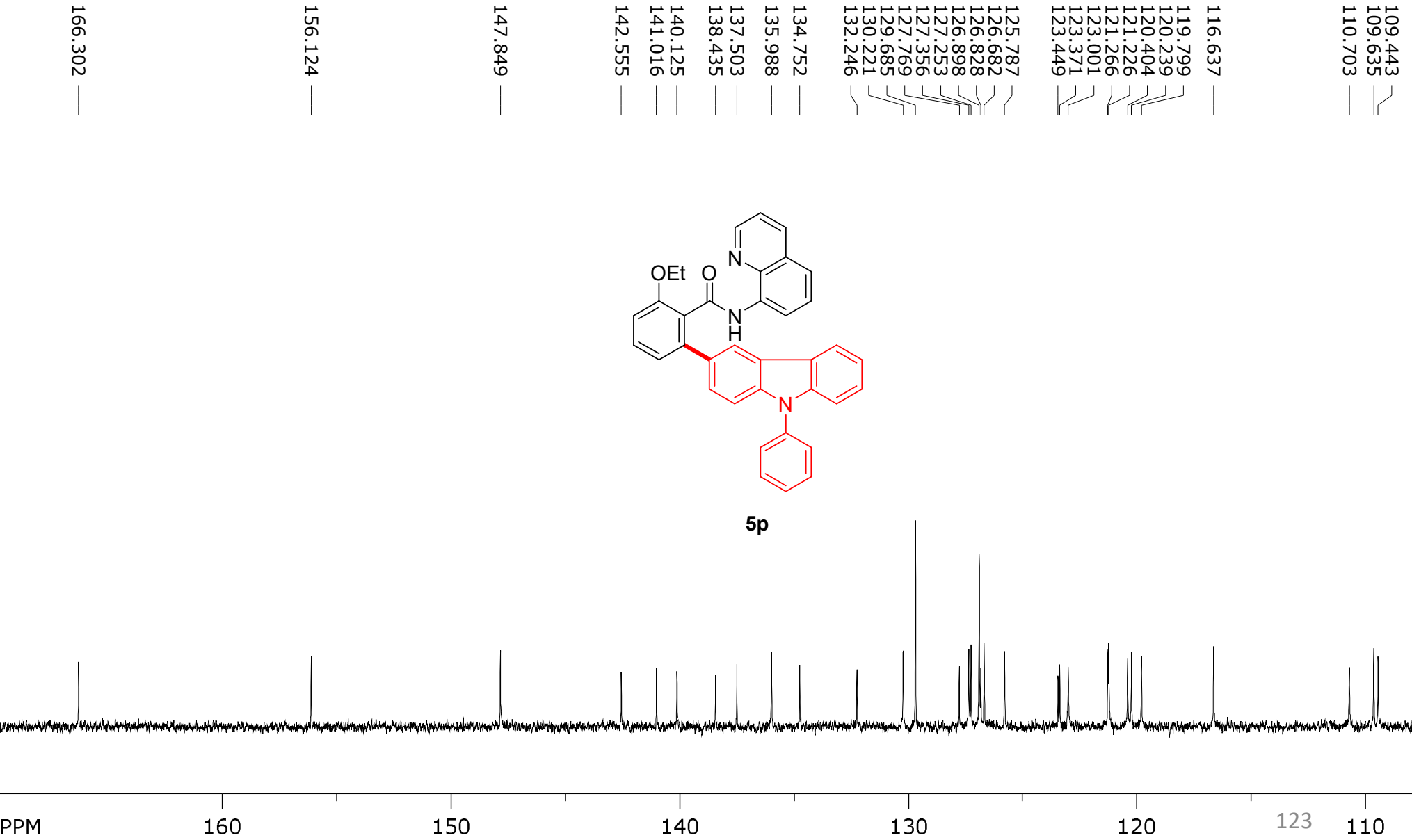
5p



SpinWorks 4: RD 721
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



SpinWorks 4: RD 721
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



SpinWorks 4: RD-2024-RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

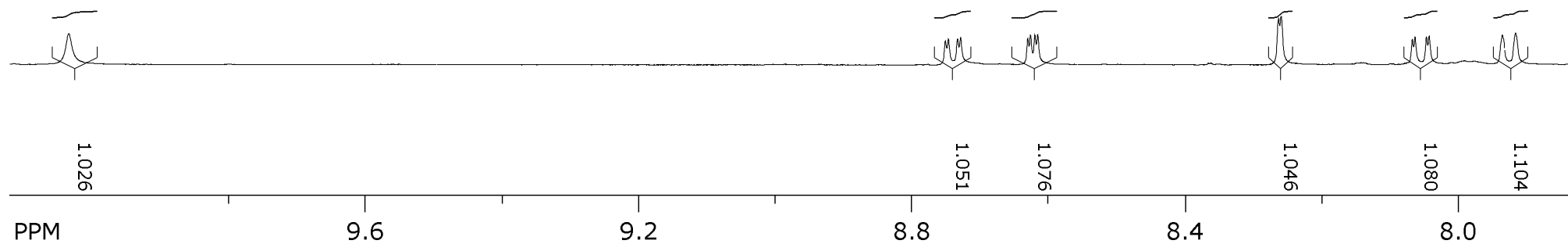
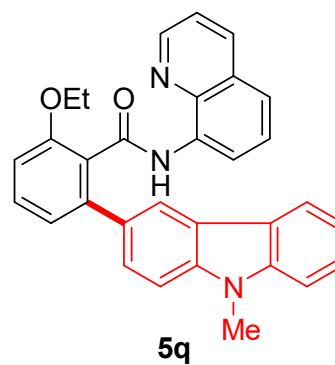
10.0349

8.6154
8.6195
8.6259
8.6300
8.7283
8.7329
8.7462
8.7507

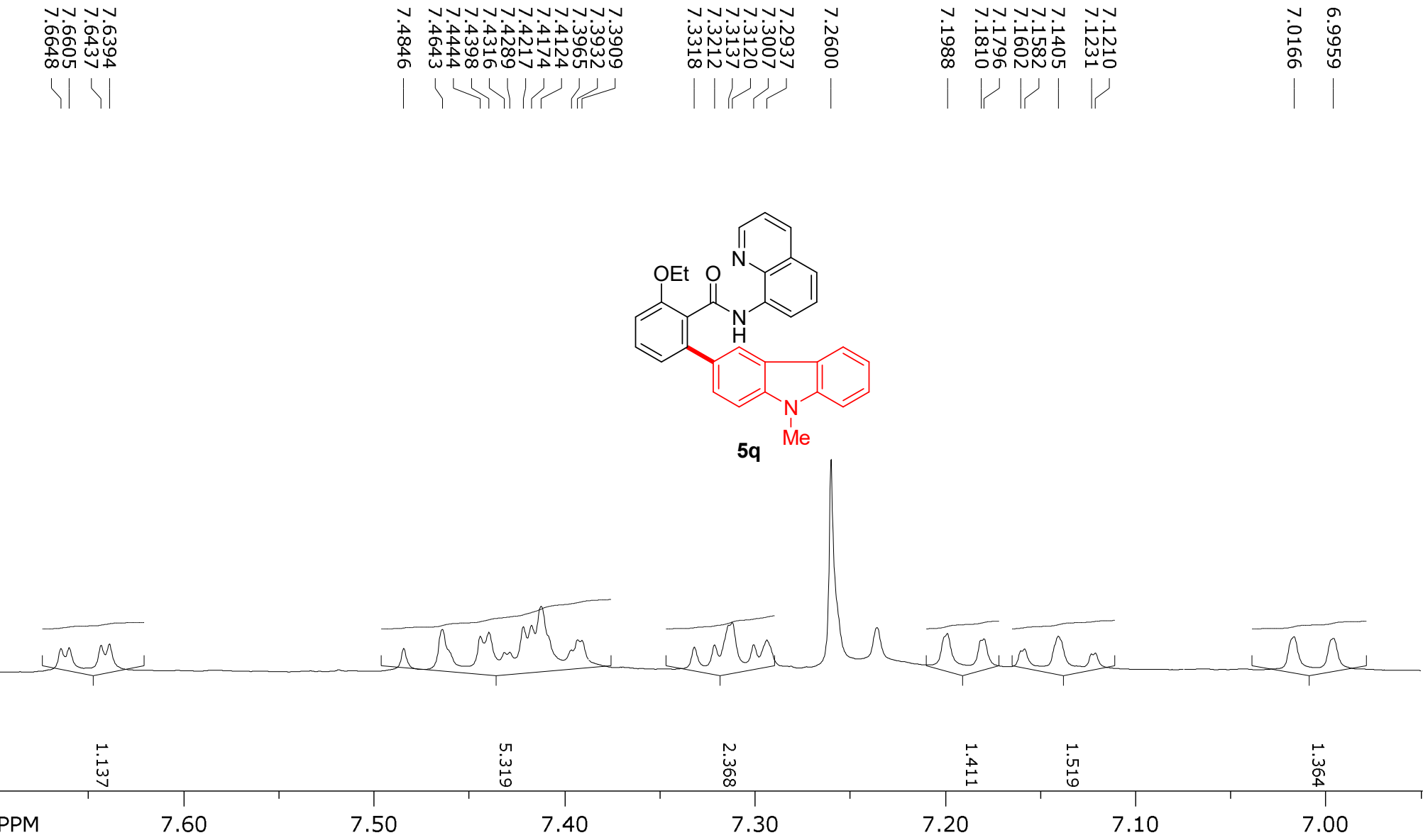
8.2588
8.2624

8.0419
8.0459
8.0625
8.0666

7.9153
7.9346



SpinWorks 4: RD-2024-RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

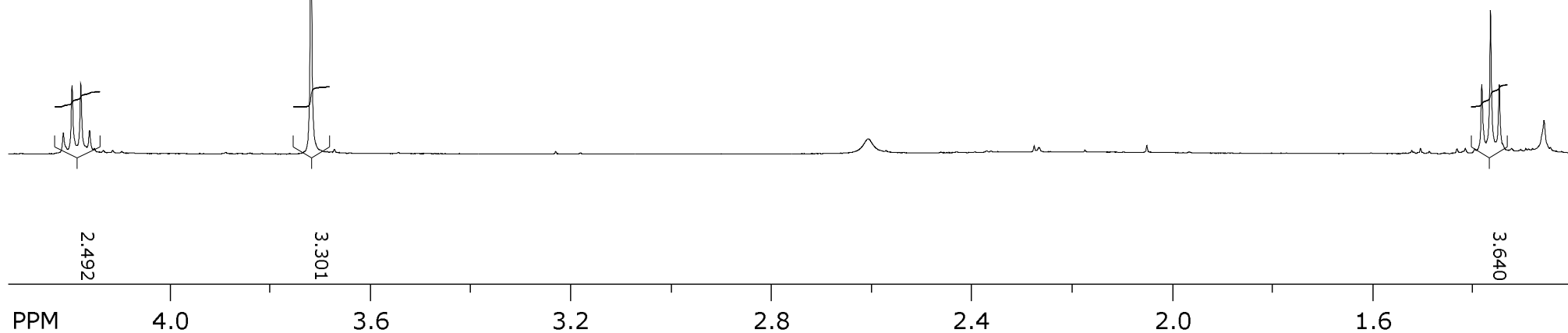
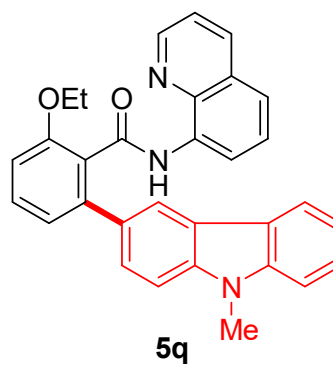


SpinWorks 4: RD-2024-RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

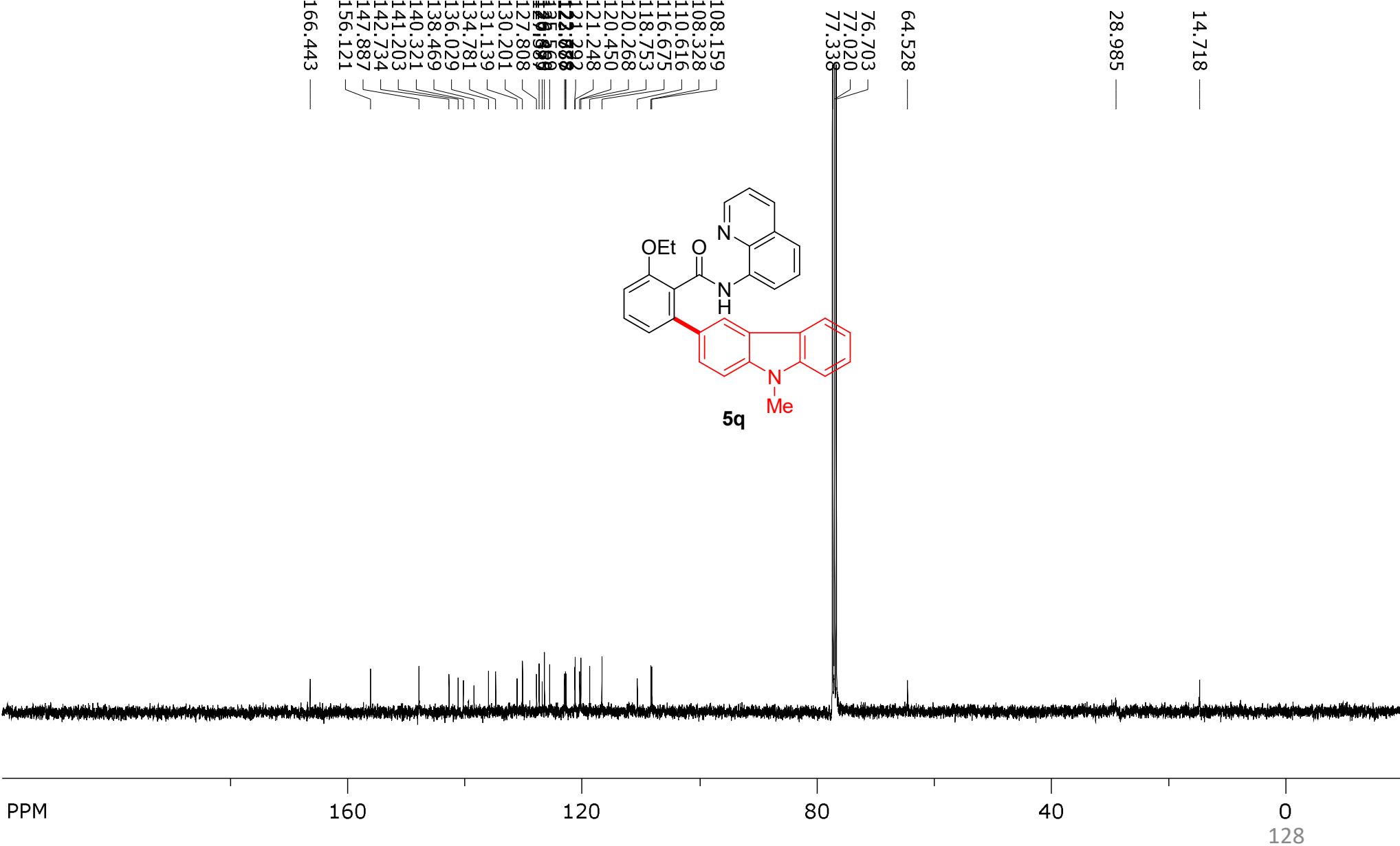
4.1614
4.1789
4.1963
4.2138

3.7195

1.3466
1.3640
1.3814

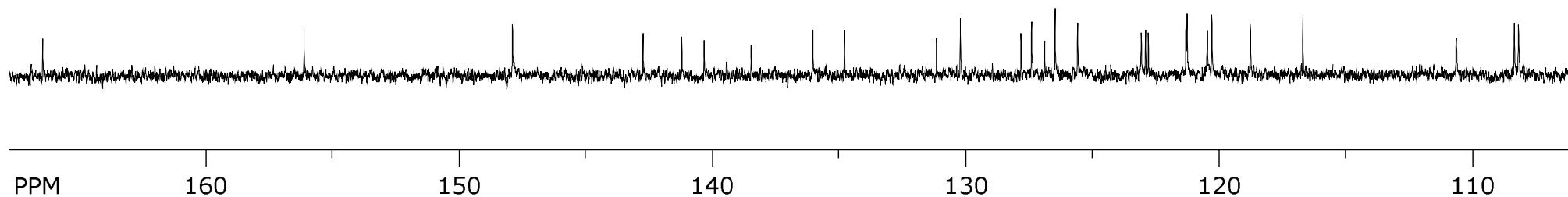
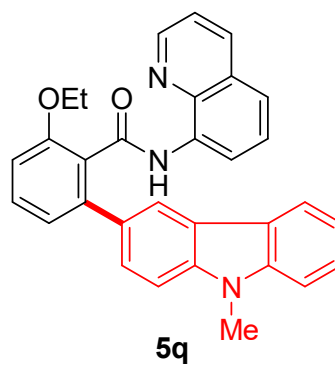


SpinWorks 4: RD-2024-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

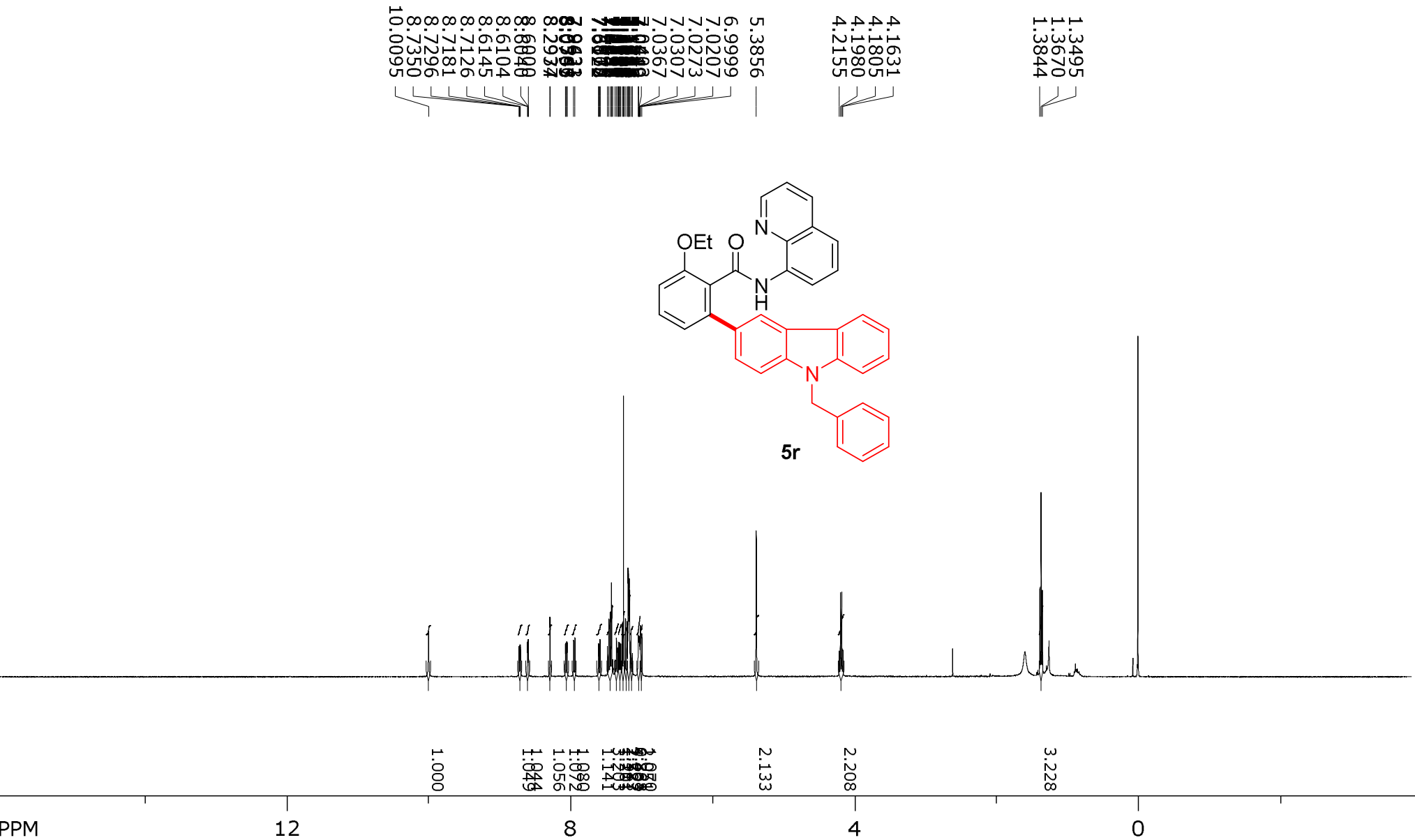


SpinWorks 4: RD-2024-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

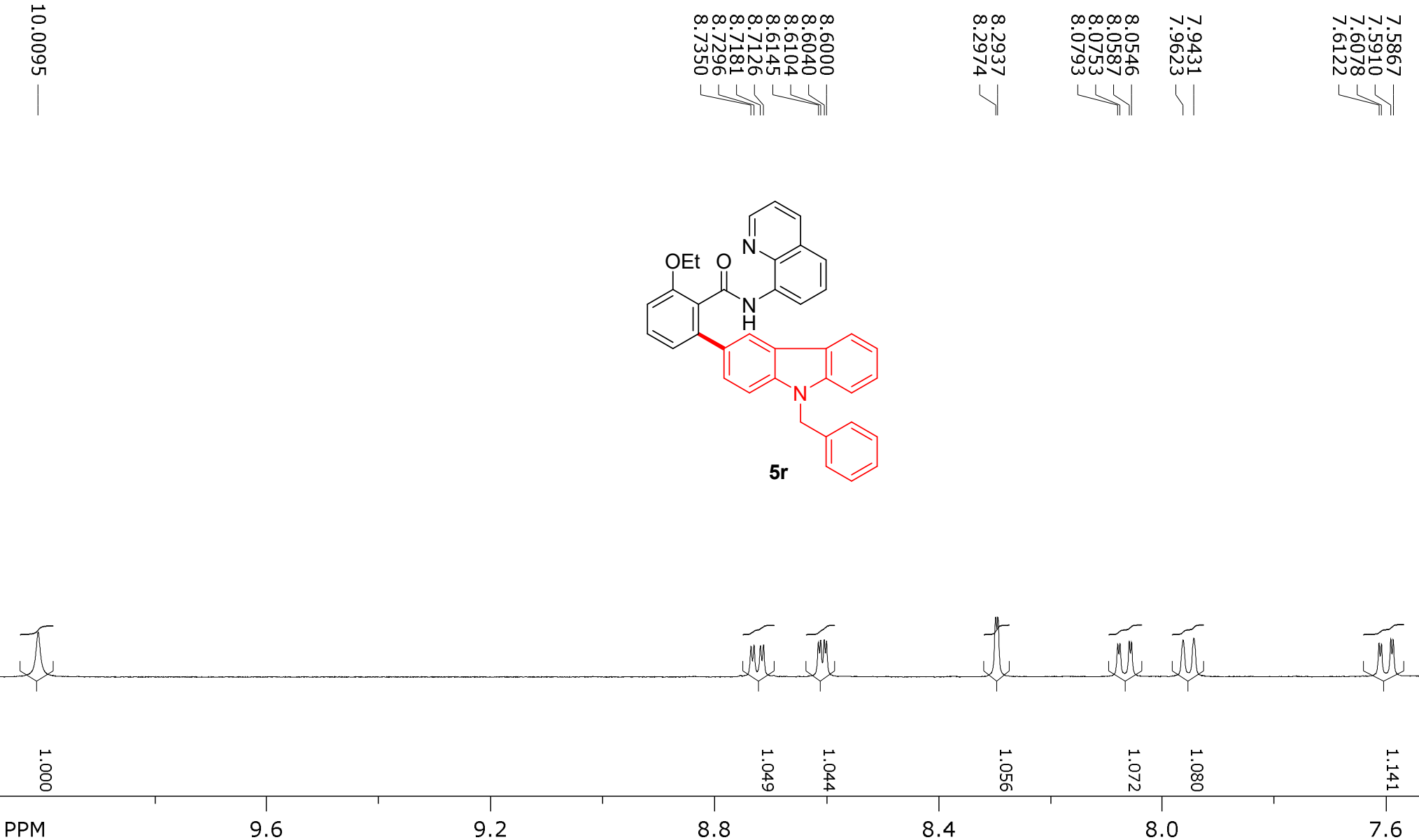
166.443 —
156.121 —
147.887 —
142.734 —
141.203 —
140.321 —
138.469 —
136.029 —
134.781 —
131.139 —
130.201 —
127.808 —
127.387 —
126.875 —
126.460 —
125.569 —
123.057 —
122.778 —
122.888 —
121.292 —
121.248 —
120.450 —
120.268 —
118.753 —
116.675 —
110.616 —
108.328 —
108.159 —



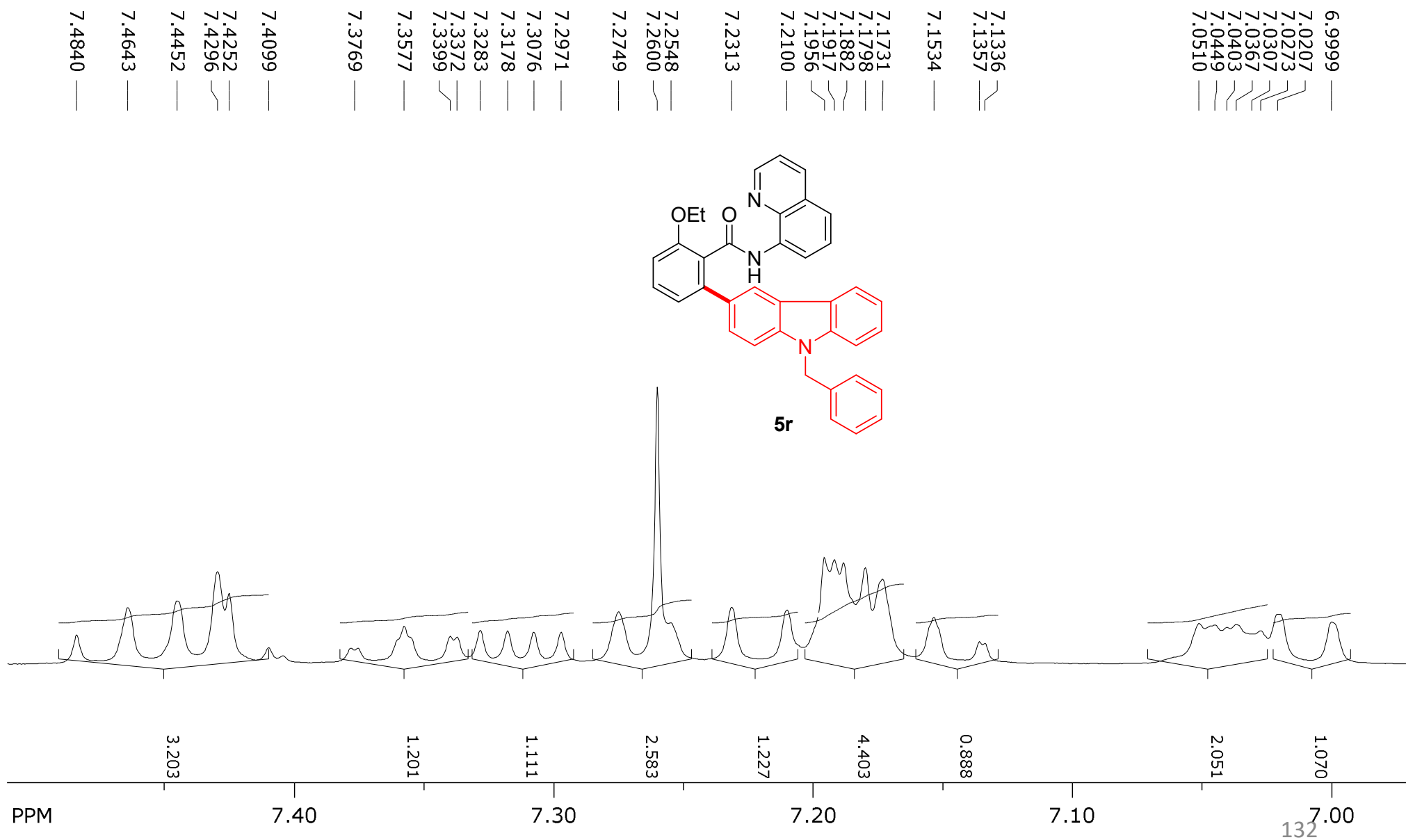
SpinWorks 4: rd-327a



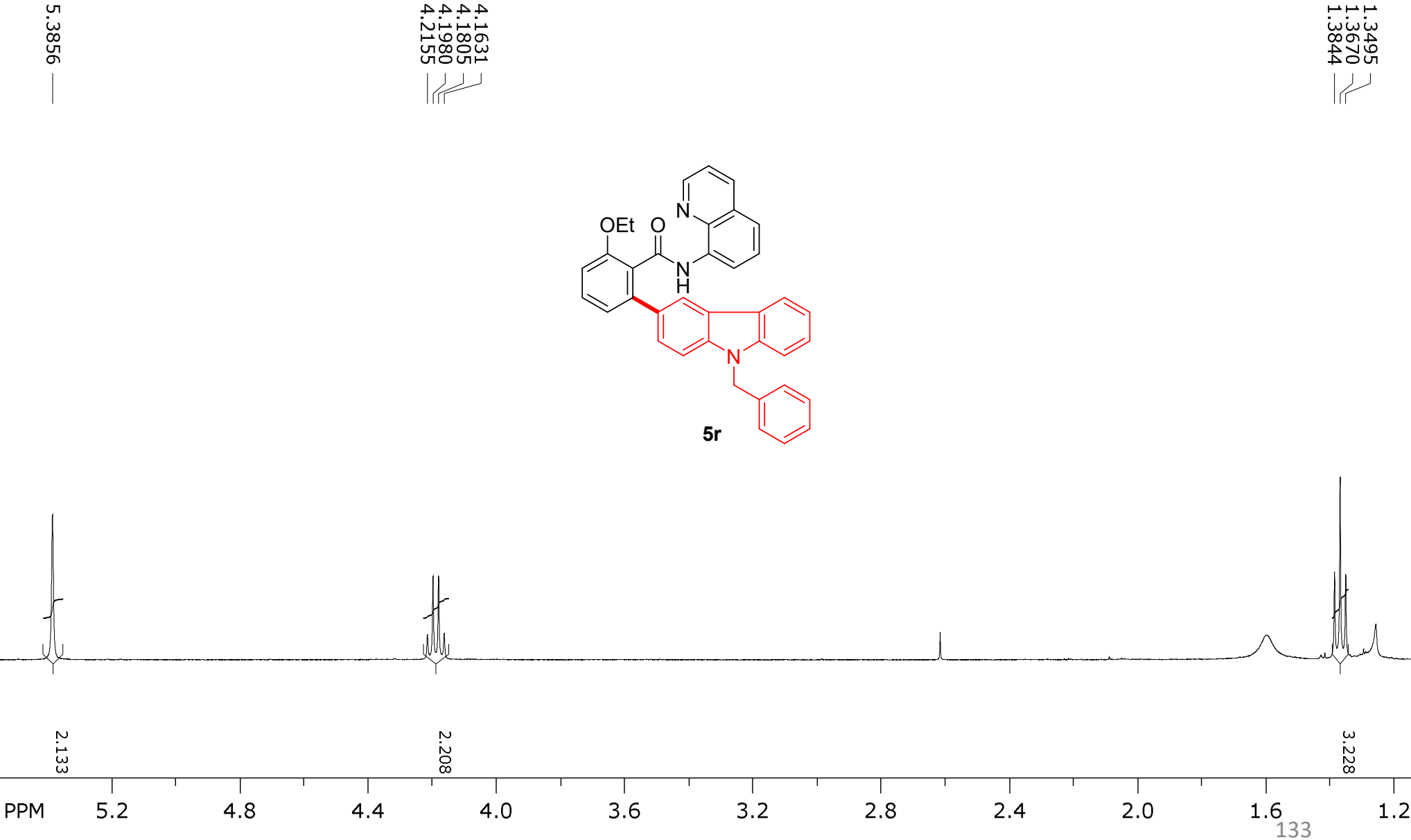
SpinWorks 4: rd-327a



SpinWorks 4: rd-327a

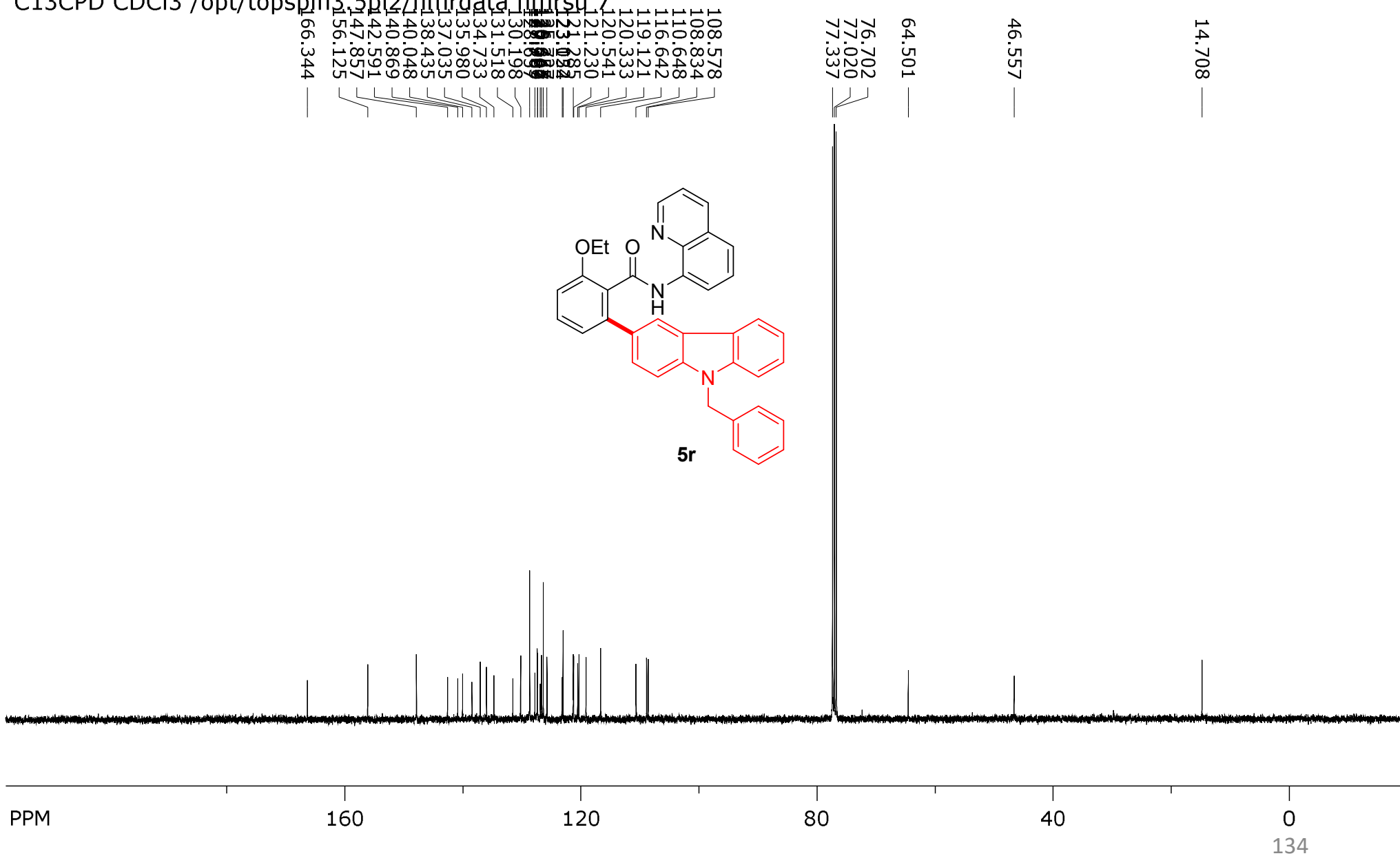


SpinWorks 4: rd-327a

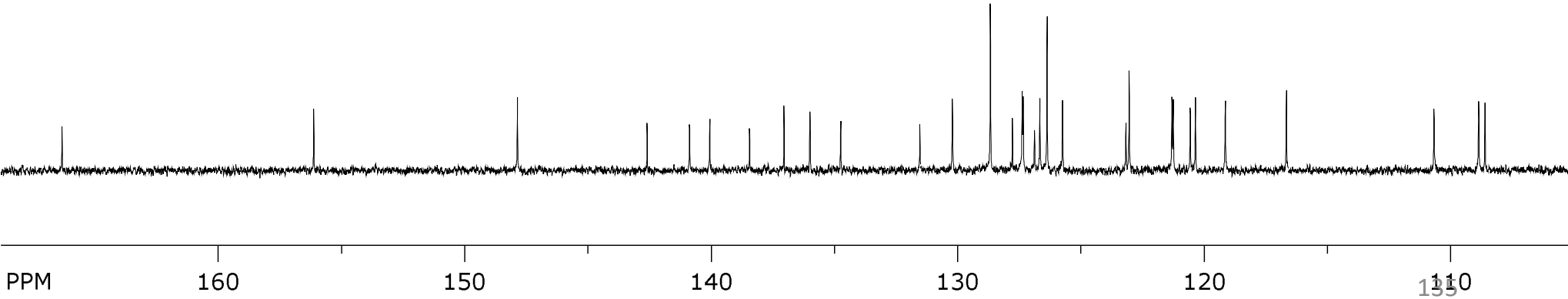
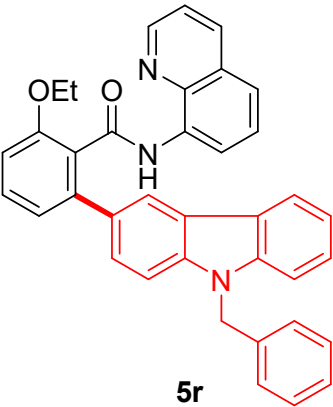
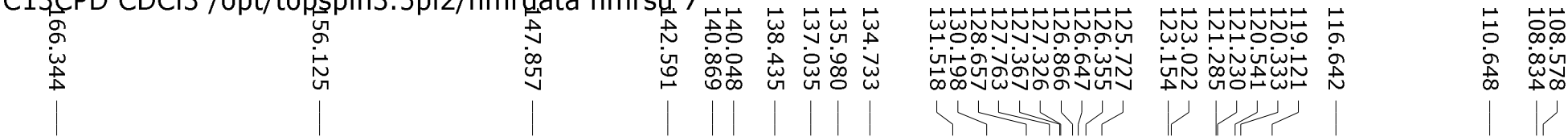


SpinWorks 4: RD 327 A

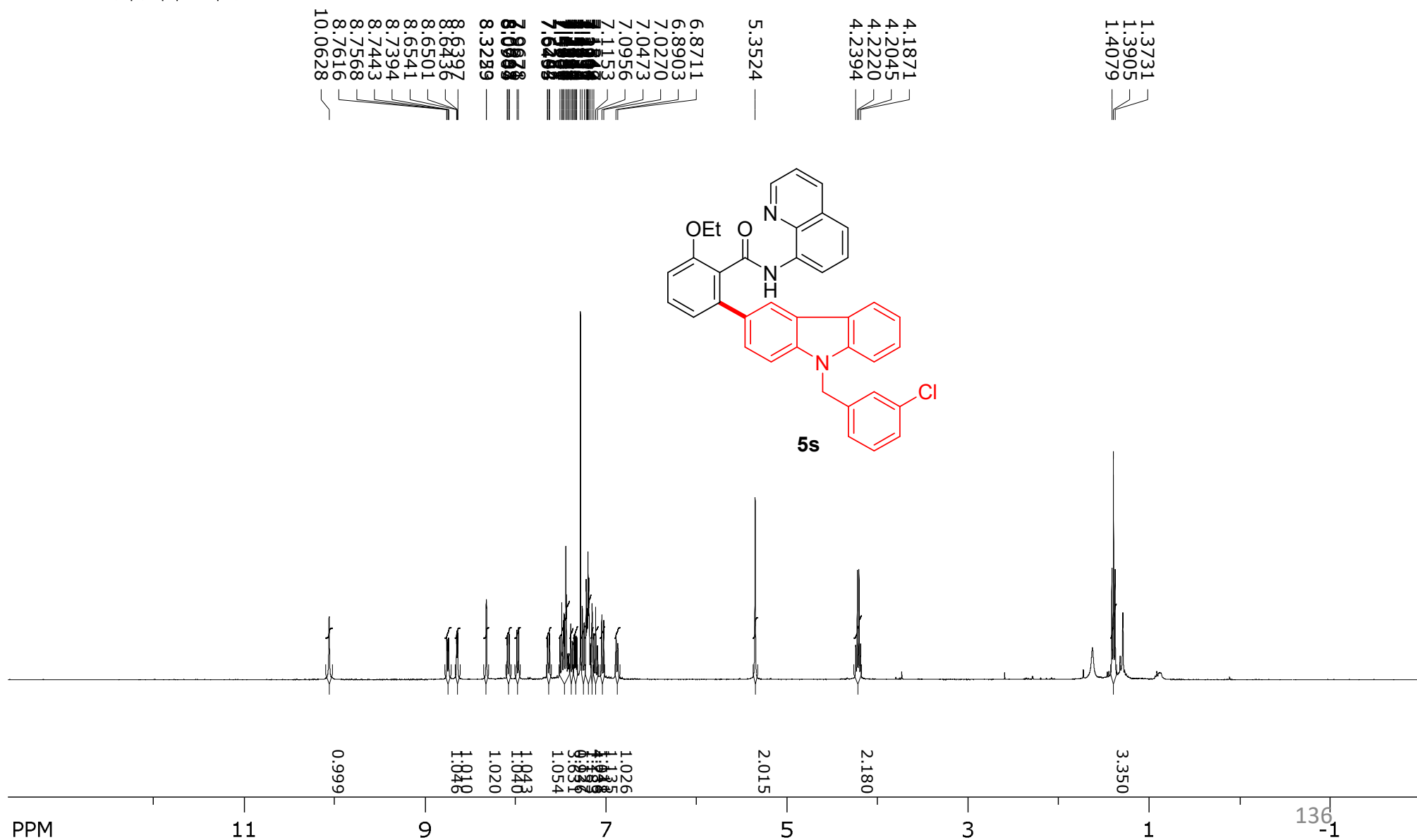
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7



SpinWorks 4: RD 327 A
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: RD-984
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

8.7394
8.7443
8.7568
8.7616

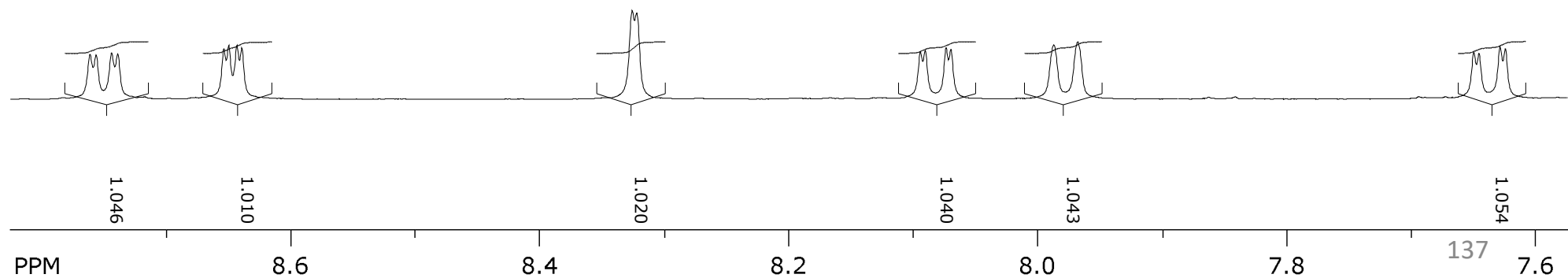
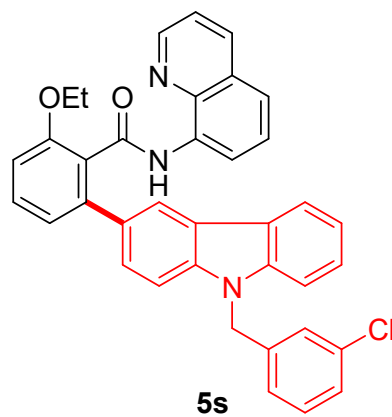
8.6397
8.6436
8.6501
8.6541

8.3223
8.3259

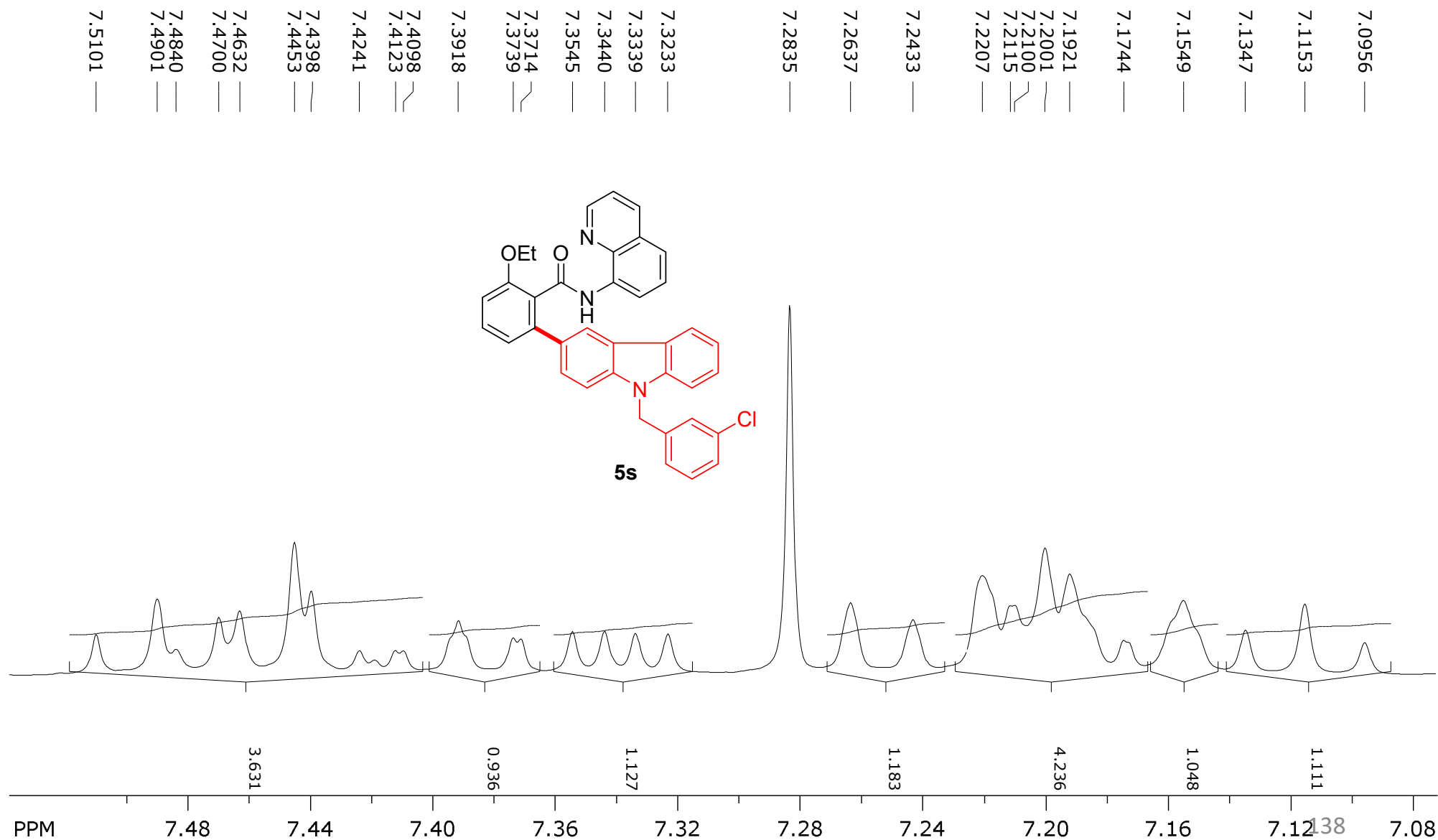
8.0698
8.0737
8.0904
8.0943

7.9678
7.9871

7.6242
7.6284
7.6453
7.6495



SpinWorks 4: RD-984
 PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



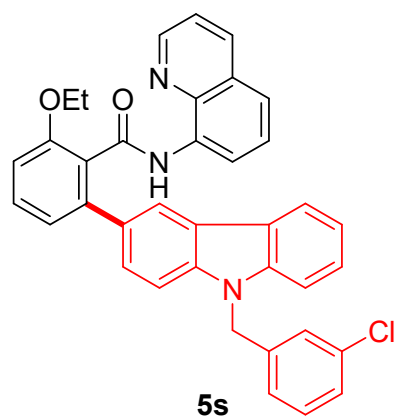
SpinWorks 4: RD-984
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

7.0473

7.0270

6.8903

6.8711



1.135

1.026

139

PPM

7.04

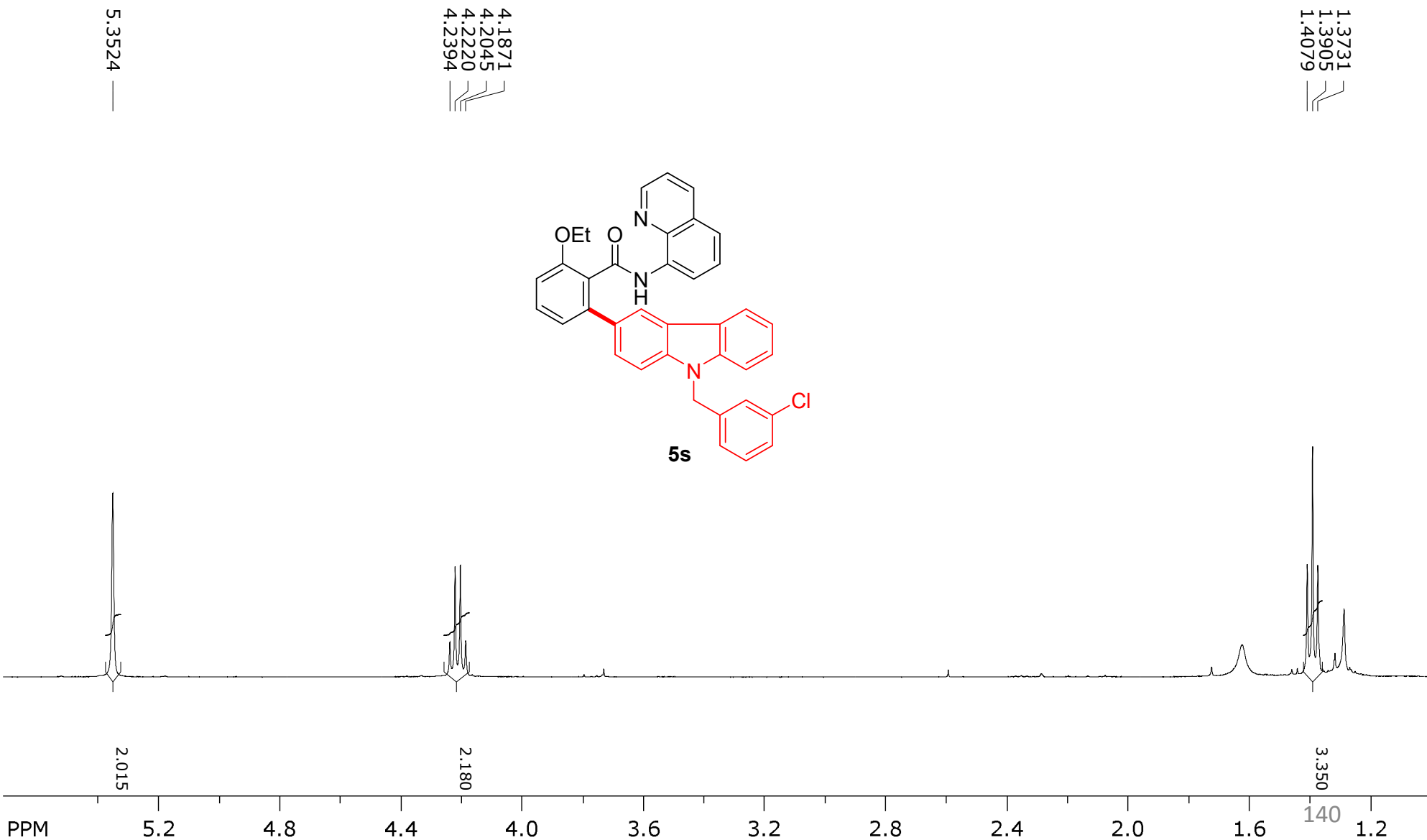
7.00

6.96

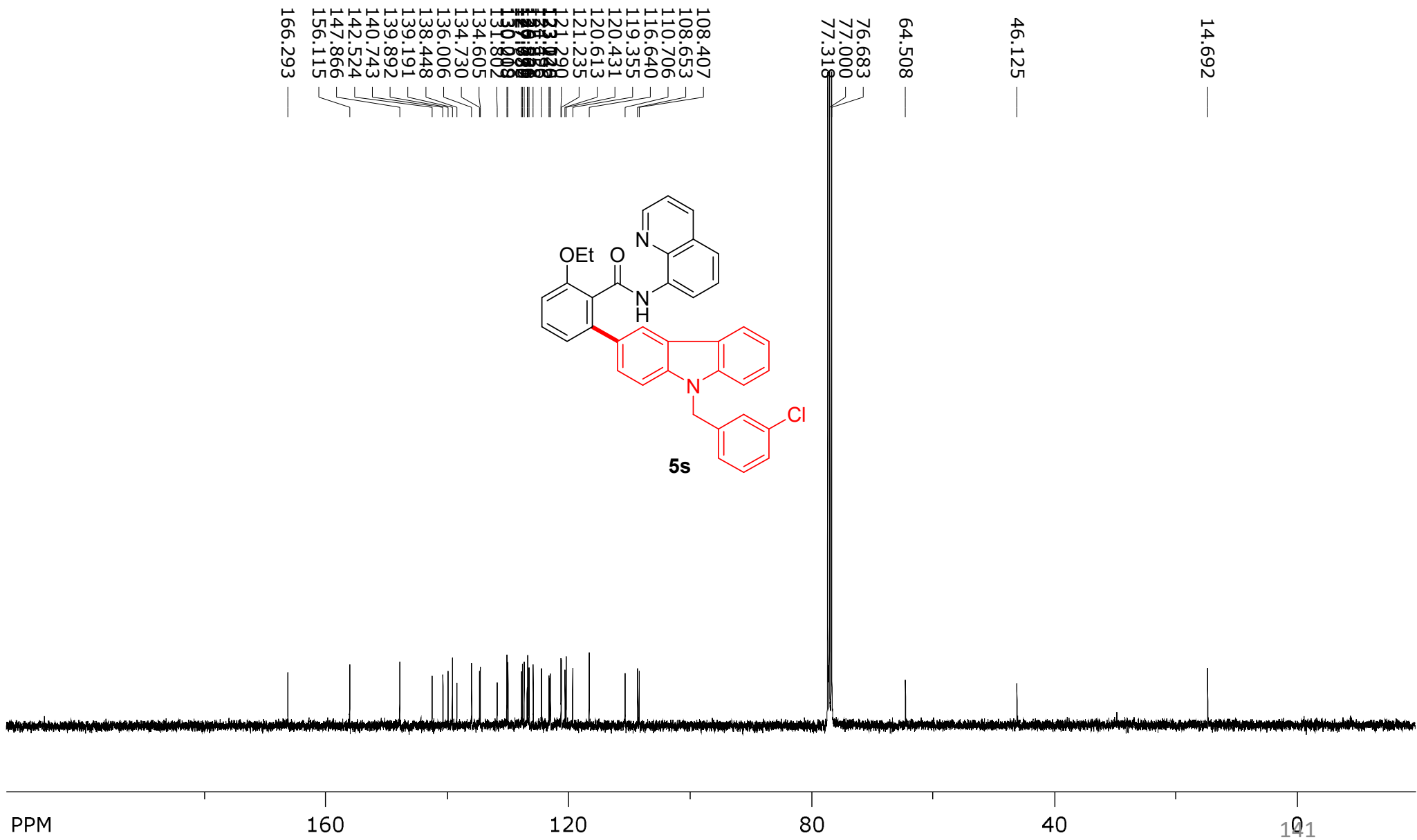
6.92

6.88

SpinWorks 4: RD-984
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

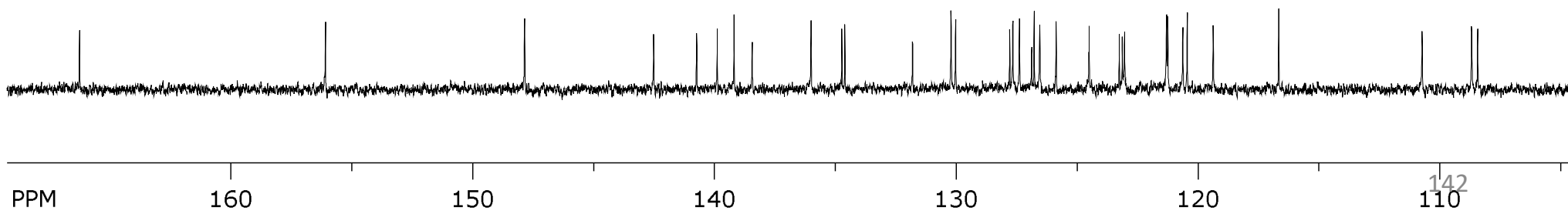
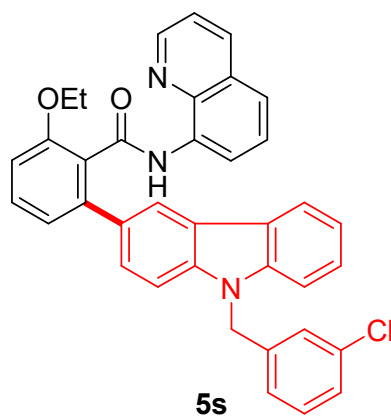


SpinWorks 4: RD-984
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

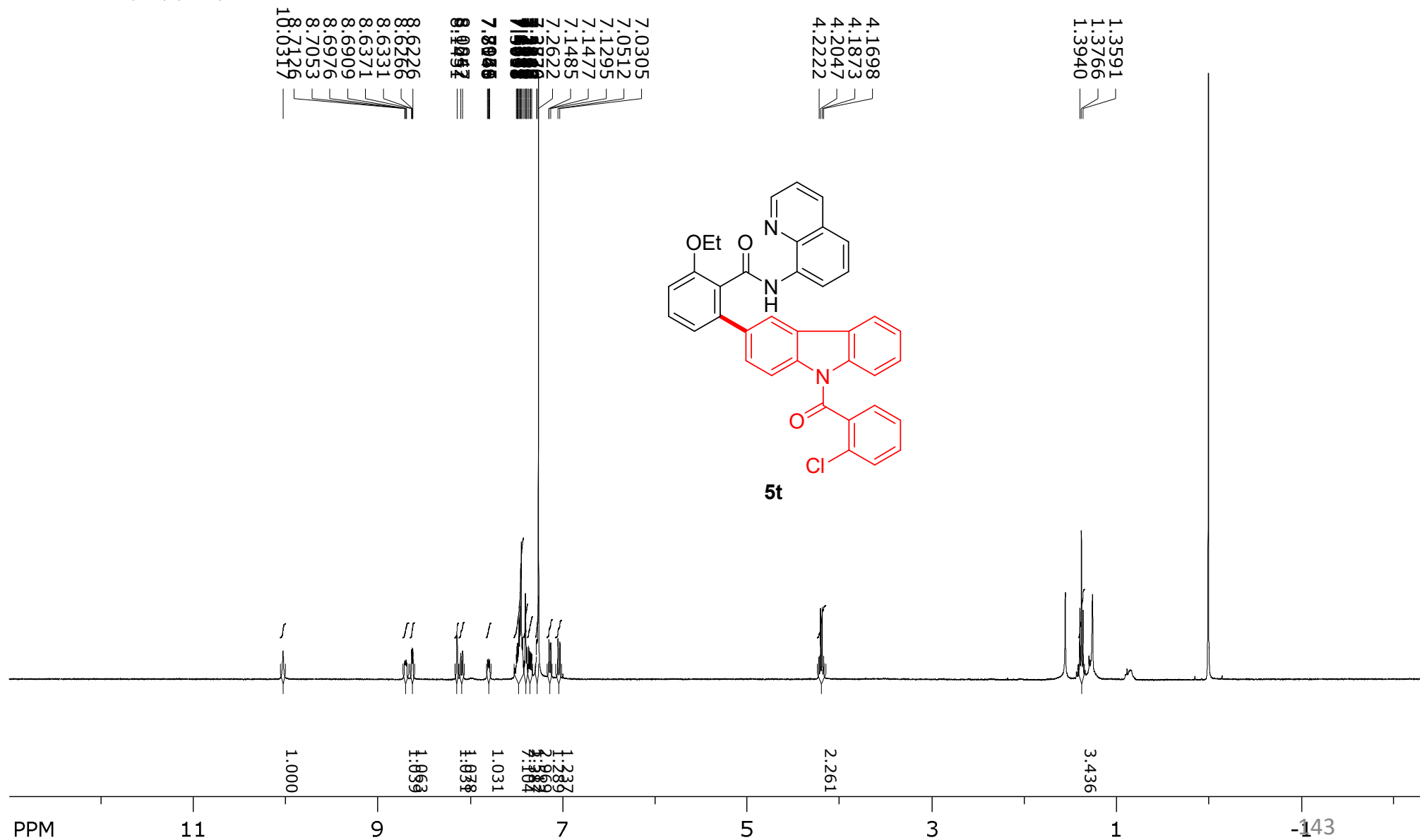


SpinWorks 4: RD-984
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

166.293	156.115	147.866	142.524	140.743	139.892	139.191	138.448	136.006	134.730	134.605	131.802	130.208	130.019	127.780	127.652	127.375	126.871	126.766	126.536	125.858	124.496	123.245	123.120	123.026	121.290	121.235	120.613	120.431	119.355	116.640	110.706	108.653	108.407
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SpinWorks 4: RD 954
 PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60

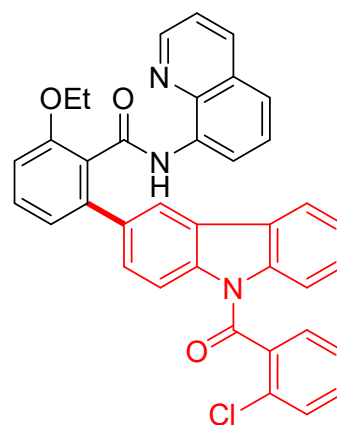


SpinWorks 4: RD 954
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60

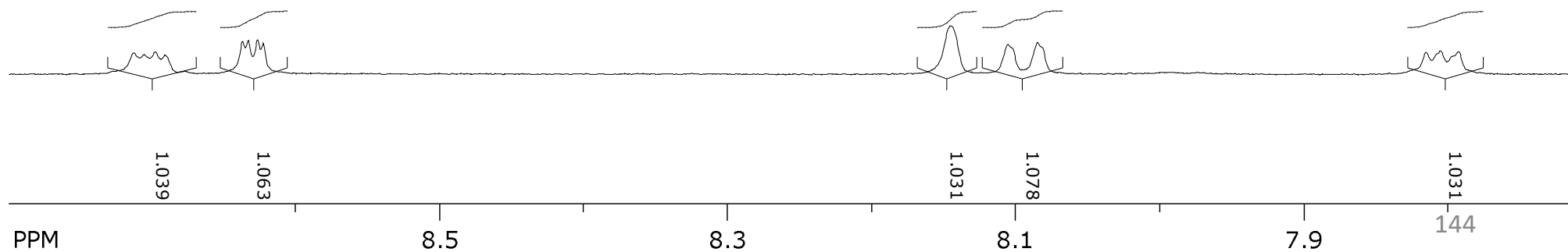
8.6226
8.6266
8.6331
8.6371
8.6909
8.6976
8.7053
8.7126

8.0847
8.1052
8.1451

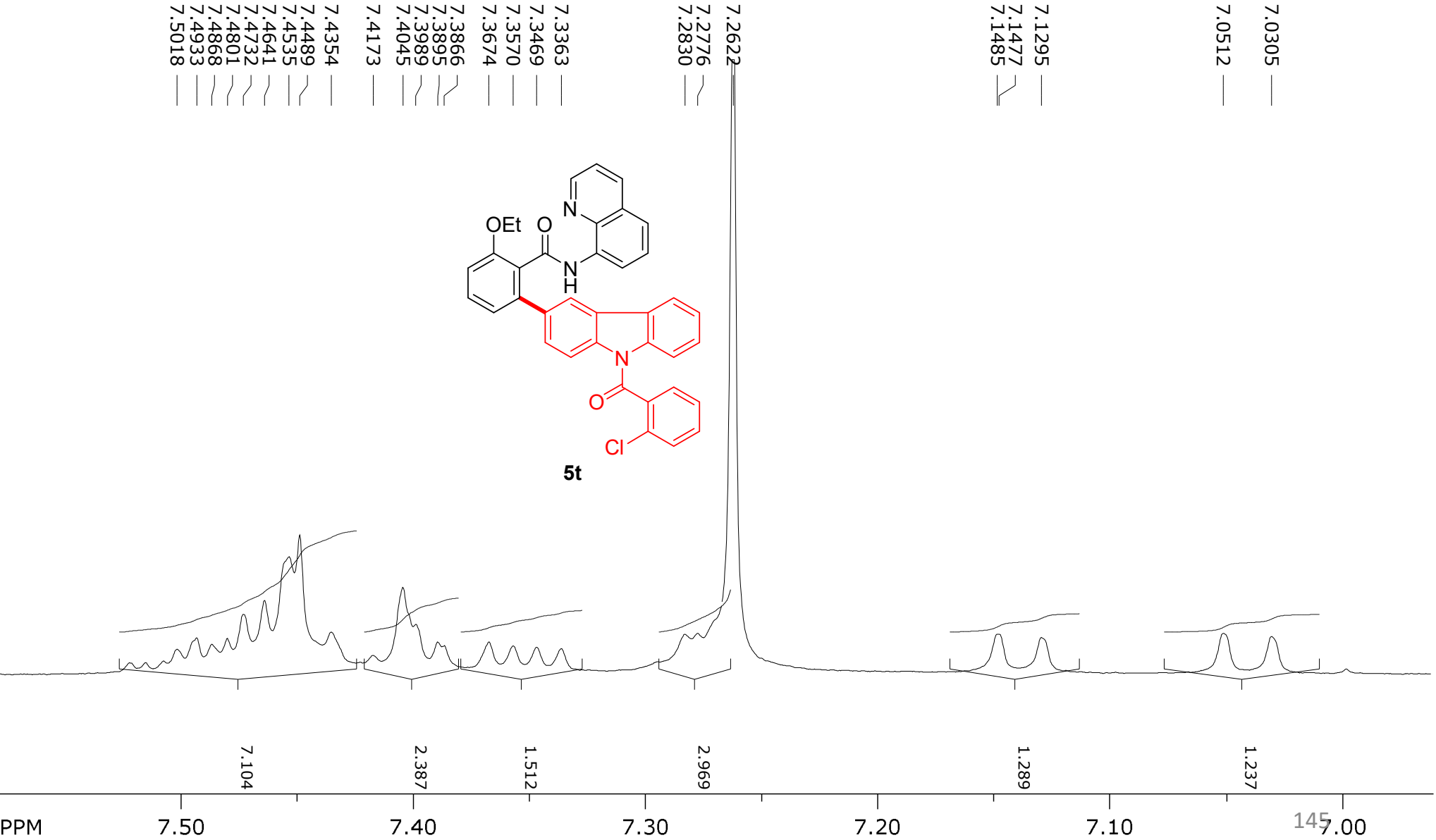
7.7921
7.7955
7.7966
7.8049
7.8148



5t



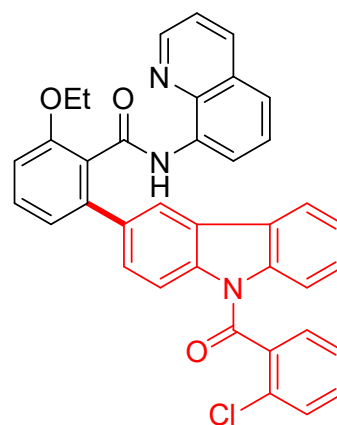
SpinWorks 4: RD 954
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



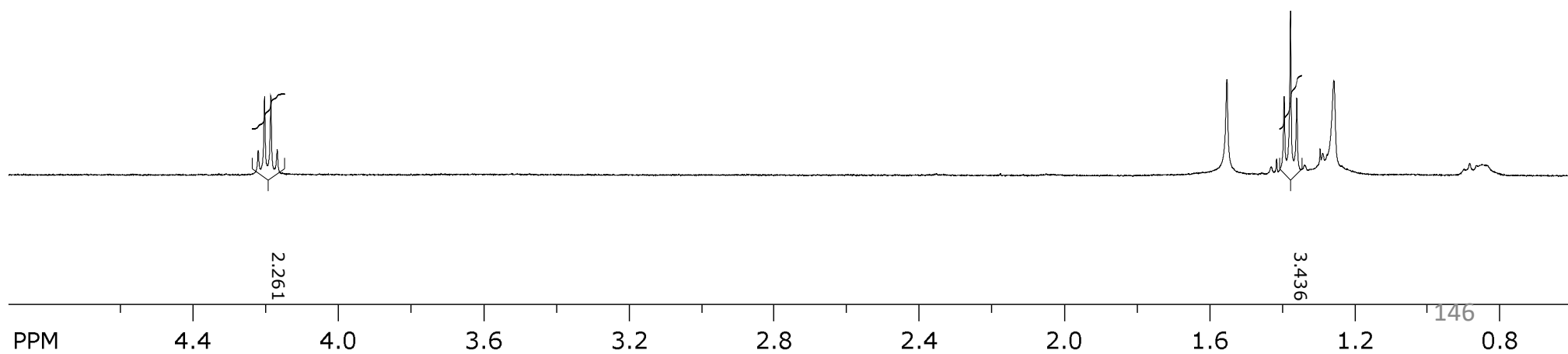
SpinWorks 4: RD 954
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60

4.1698
4.1873
4.2047
4.2222

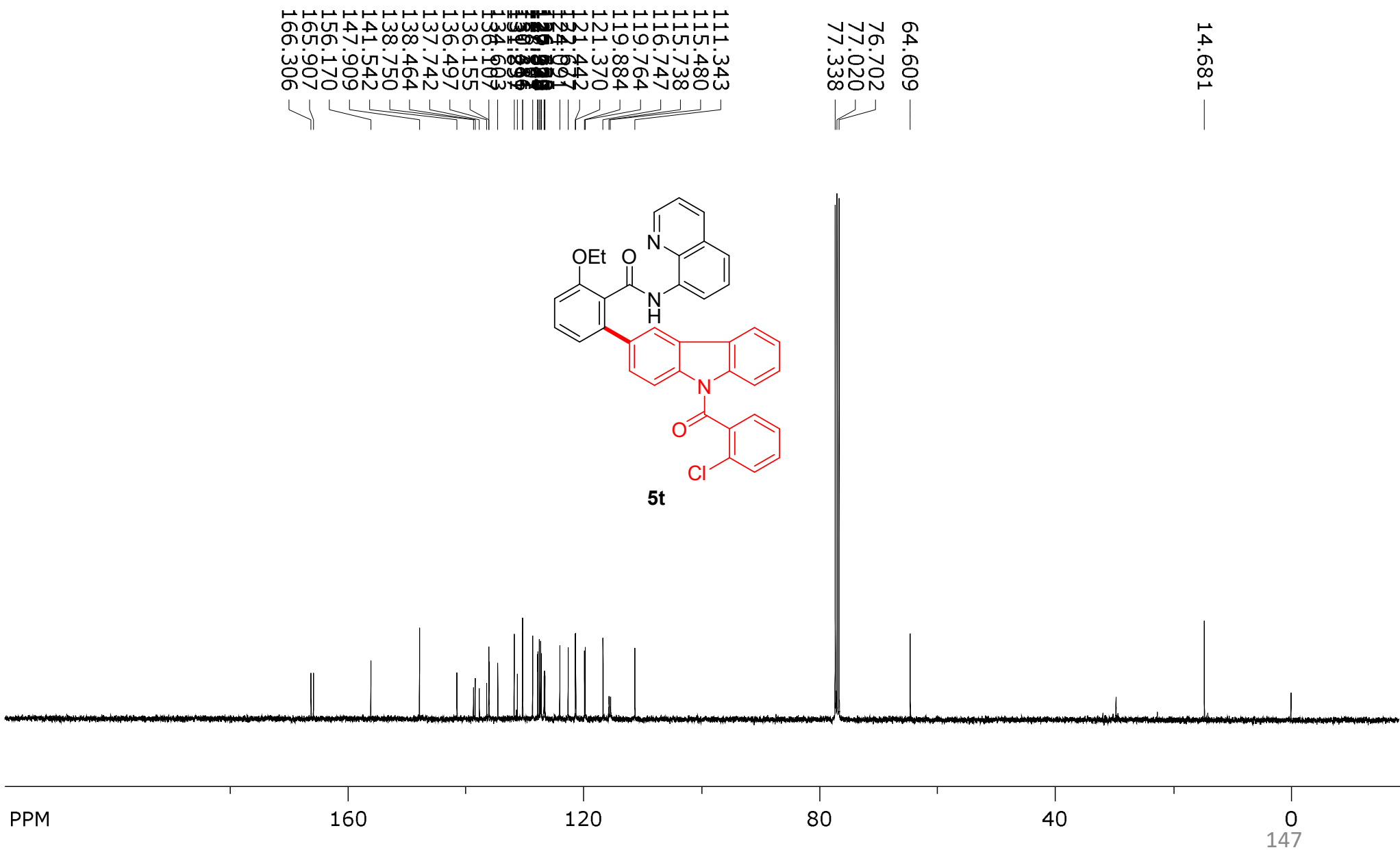
1.3591
1.3766
1.3940



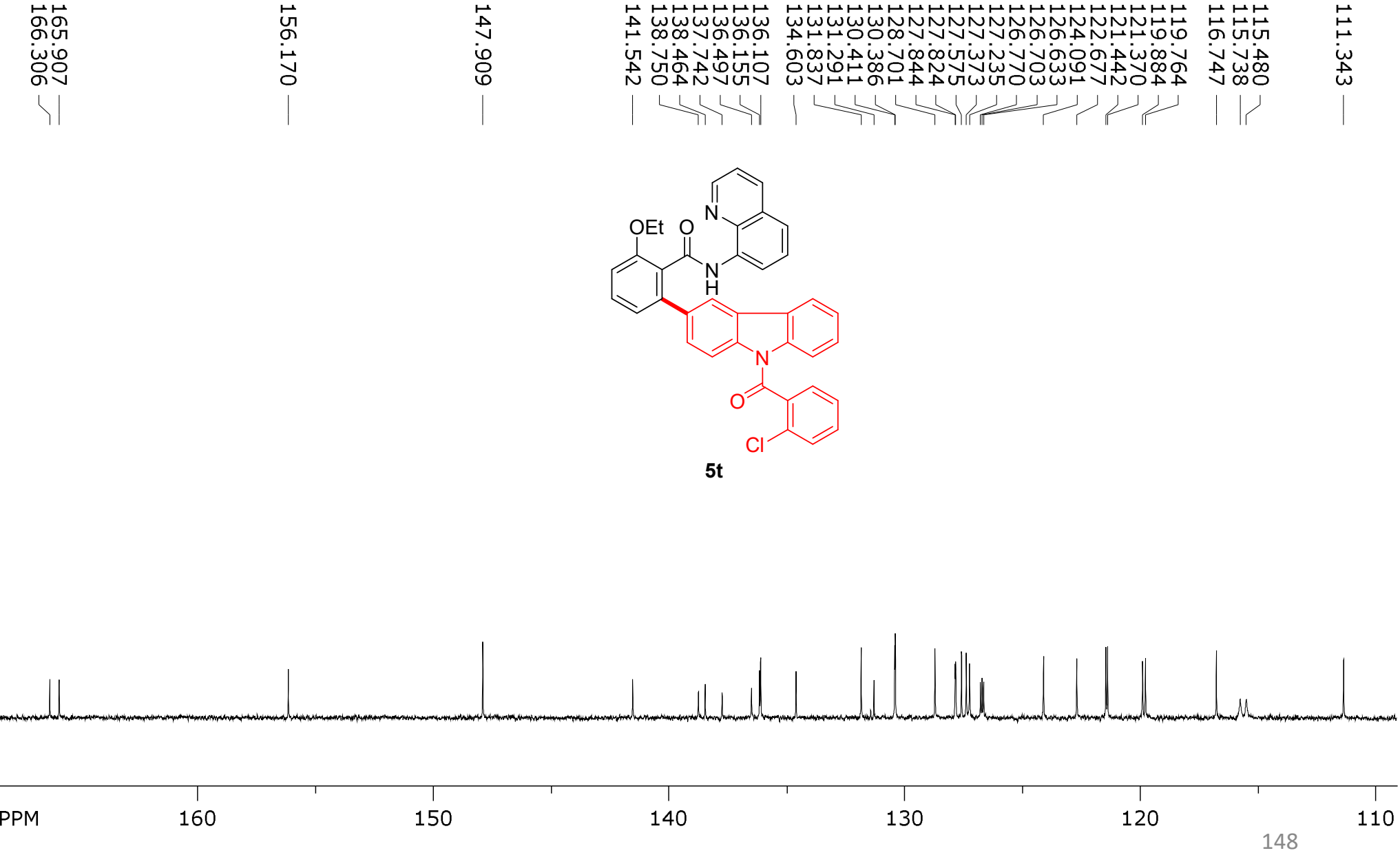
5t



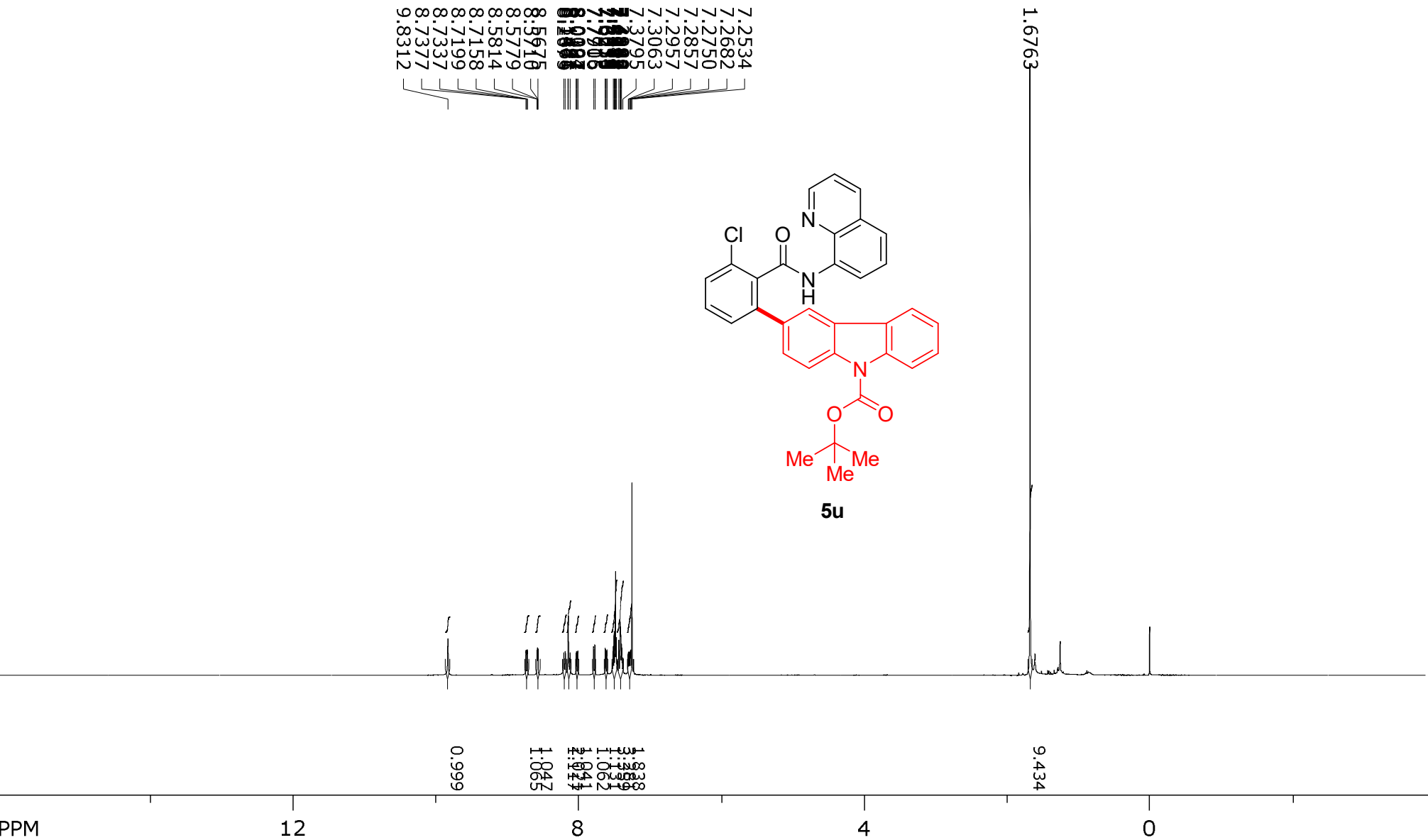
SpinWorks 4: RD 954



SpinWorks 4: RD 954



SpinWorks 4: RD-905
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30



SpinWorks 4: RD-905
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30



SpinWorks 4: RD-905
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30

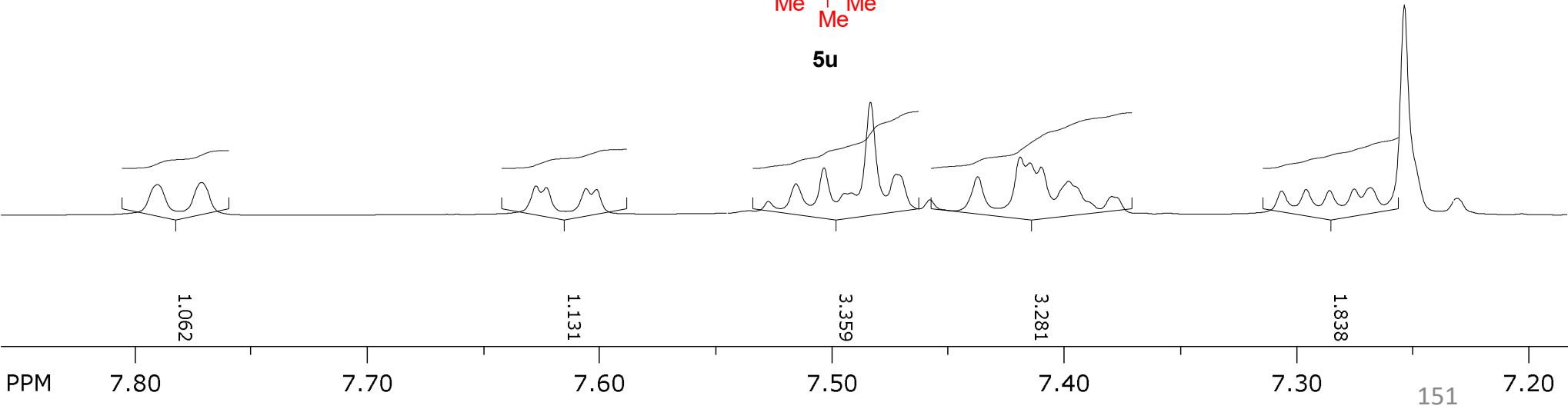
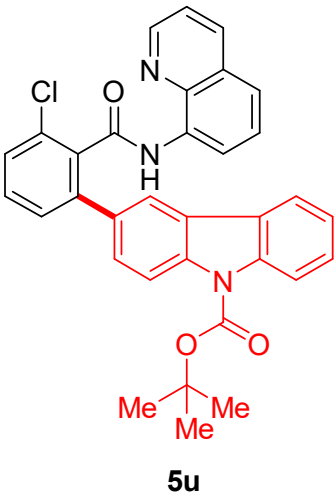
7.7715 —
7.7906 —

7.6014 —
7.6059 —
7.6230 —
7.6275 —

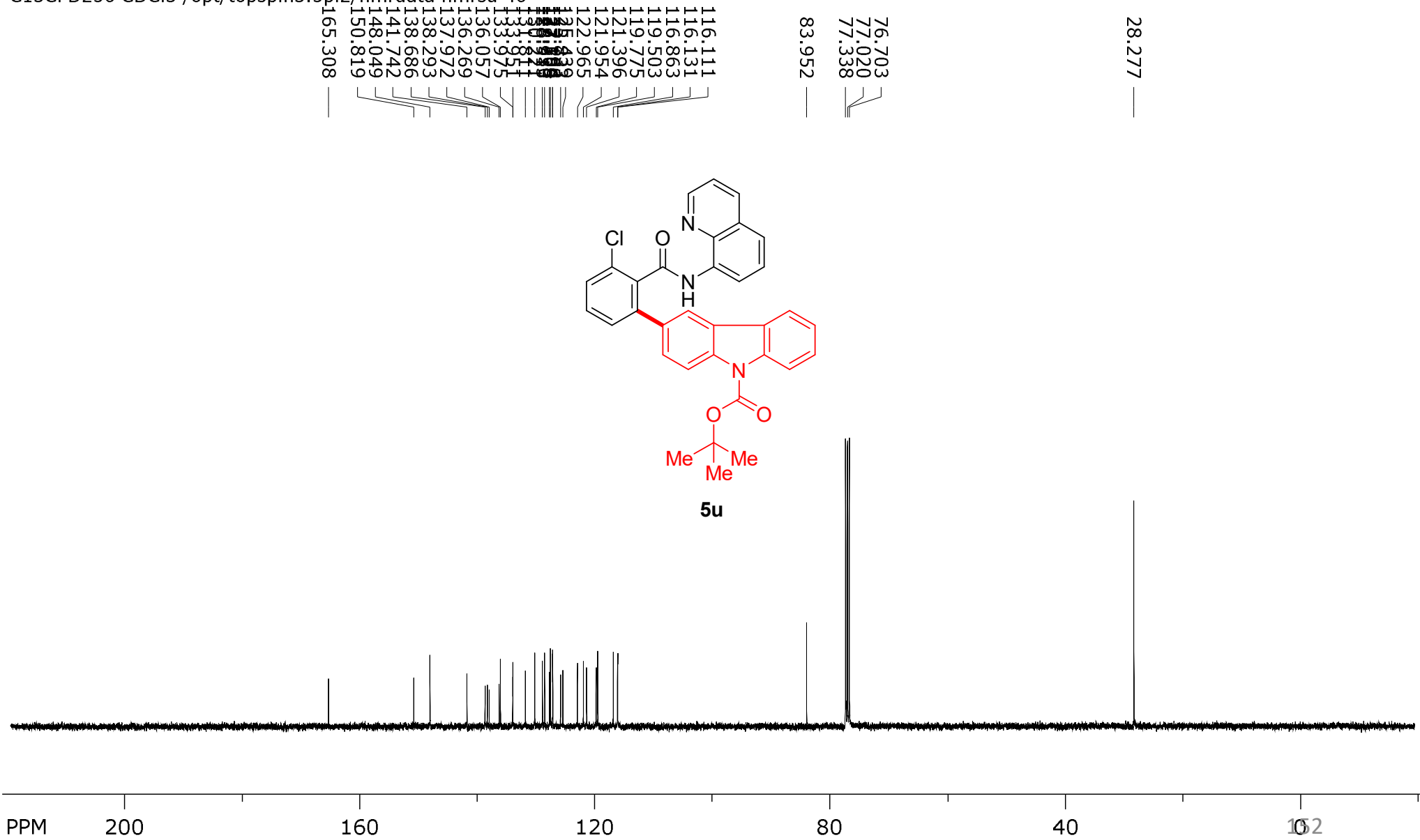
7.4723 —
7.4834 —
7.4915 —
7.4944 —
7.5034 —
7.5155 —

7.4372 —
7.4189 —
7.4147 —
7.4098 —
7.3980 —
7.3795 —

7.2534 —
7.2682 —
7.2750 —
7.2857 —
7.2957 —
7.3063 —

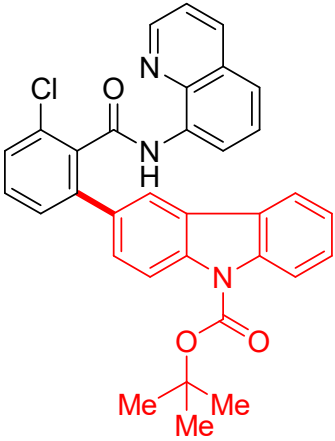


SpinWorks 4: RD 905
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 46

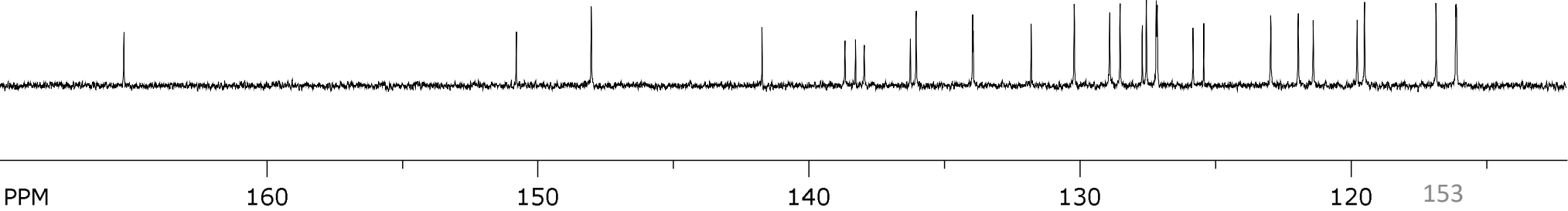


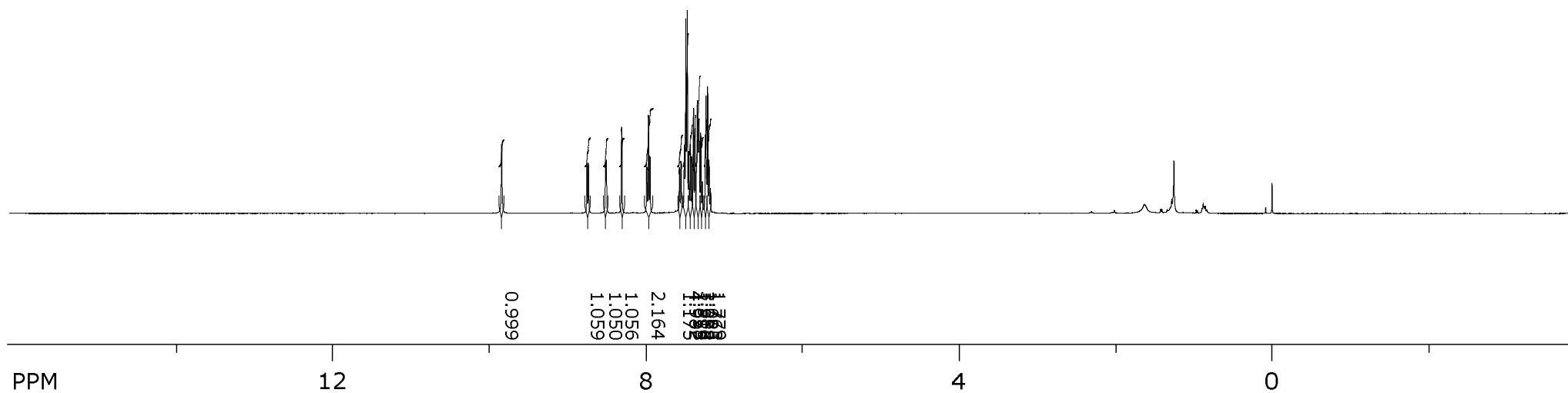
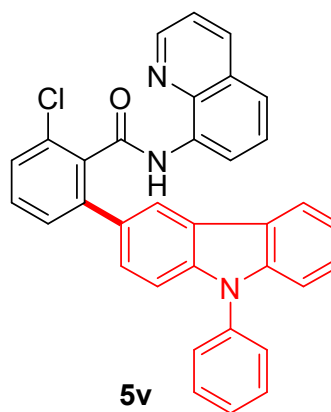
SpinWorks 4: RD 905
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 46

165.308 —
150.819 —
148.049 —
141.742 —
138.293 —
138.686 —
137.972 —
136.269 —
136.057 —
133.975 —
133.951 —
131.811 —
130.221 —
128.913 —
128.530 —
127.708 —
127.559 —
127.194 —
127.158 —
125.833 —
125.439 —
122.965 —
121.954 —
121.396 —
119.775 —
119.503 —
116.863 —
116.131 —
116.111 —



5u



$1H$ 

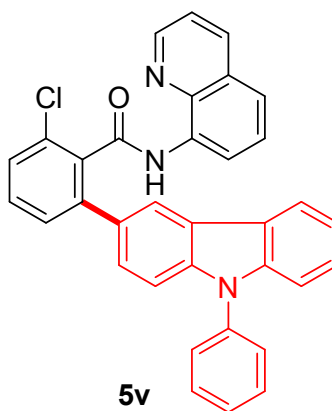
SpinWorks 4: RD291-REP-3
1H



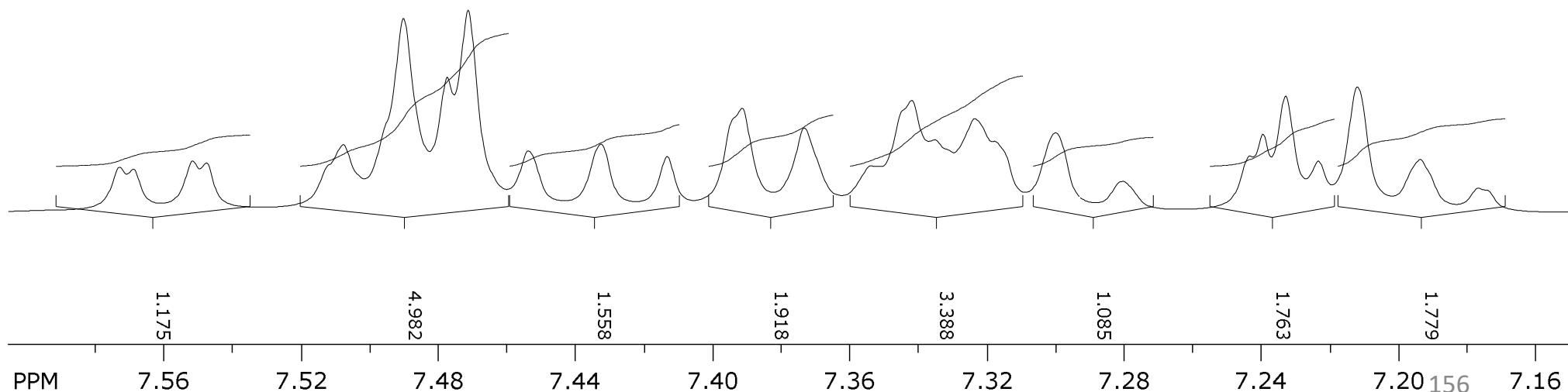
SpinWorks 4: RD291-REP-3

¹H

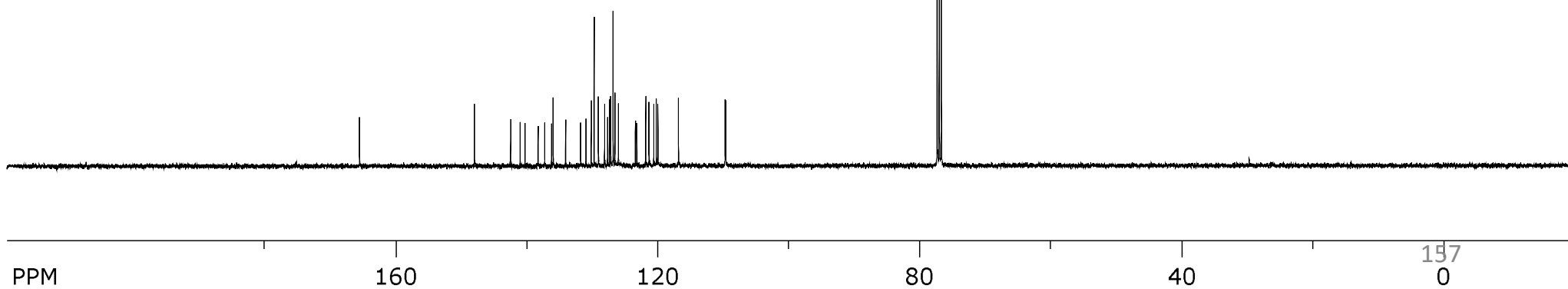
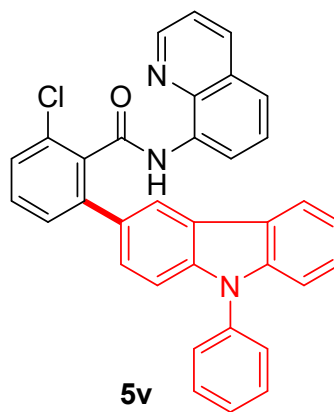
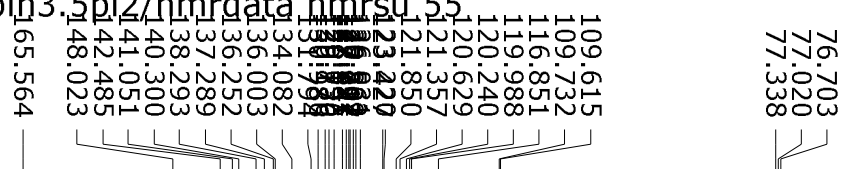
7.5691 —
7.5731 —
7.5477 —
7.5518 —
7.5078 —
7.4902 —
7.4714 —
7.4775 —
7.4538 —
7.4326 —
7.4133 —
7.3914 —
7.3733 —
7.3539 —
7.3516 —
7.3419 —
7.3352 —
7.3235 —
7.3178 —
7.2999 —
7.2804 —
7.2433 —
7.2394 —
7.2328 —
7.2233 —
7.2119 —
7.1935 —
7.1766 —



5v

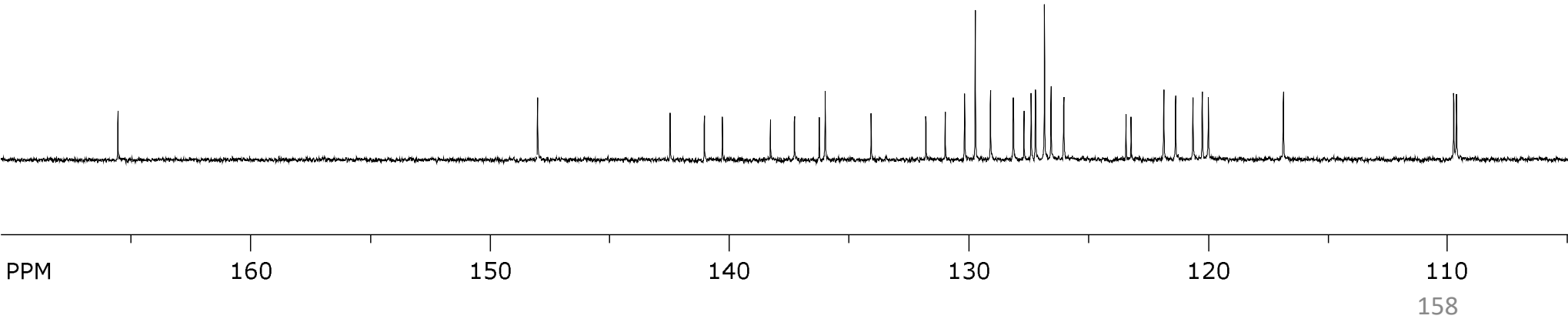
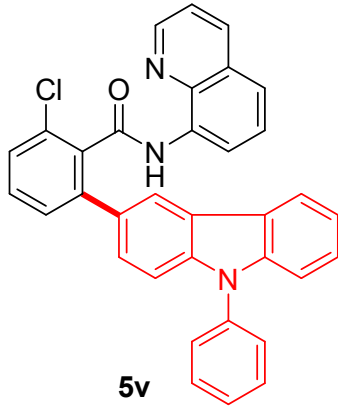


C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata/nmr50_55

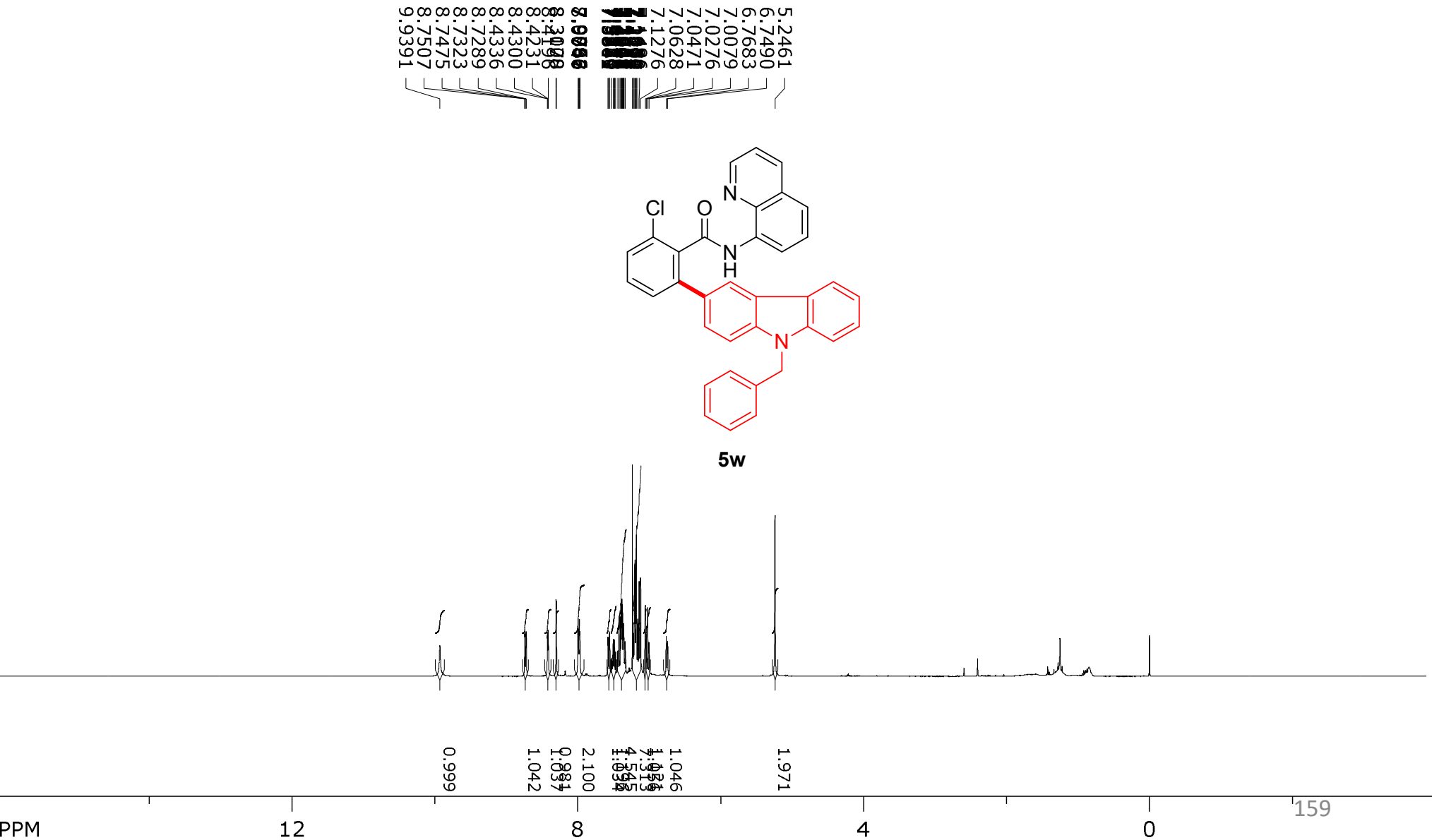


SpinWorks 4: RD 291 REP 3
C13CPD.CDCI3 /opt/topspin3.5pl2/nmrdata nmrsu 55

165.564	148.023	142.485	140.300	141.051	138.293	136.003	136.252	137.289	134.082	131.794	130.986	130.176	129.730	129.093	128.141	127.691	127.397	127.212	126.839	126.562	126.031	123.427	123.220	121.850	121.357	120.629	120.240	119.988	116.851	109.615	109.732
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SpinWorks 4: RD-1273
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20



SpinWorks 4: RD-1273
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

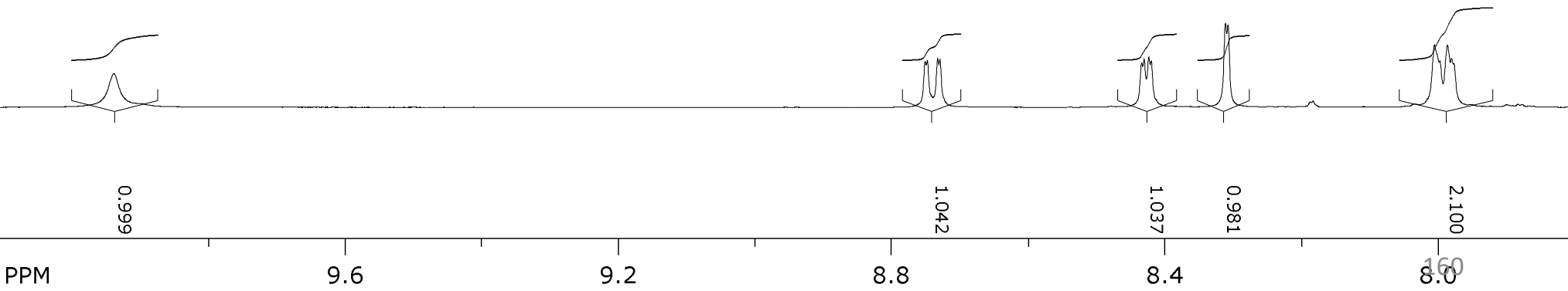
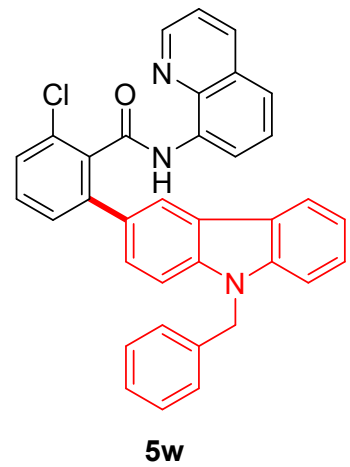
9.9391 —

8.7289
8.7323
8.7475
8.7507

8.4196
8.4231
8.4300
8.4336

8.3070
8.3108

7.9762
7.9796
7.9856
7.9967
8.0046



SpinWorks 4: RD-1273

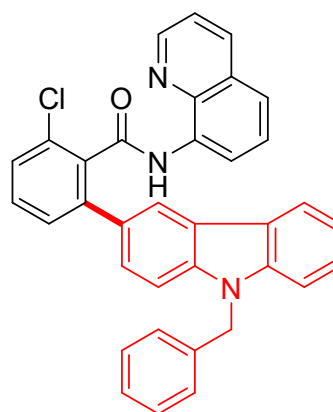
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

7.3433
7.3452
7.3631
7.3665
7.3683
7.3729
7.3815
7.3900
7.3935
7.3995
7.4097
7.4286
7.4490
7.4775
7.4918
7.4976
7.5118
7.5331
7.5589
7.5631
7.5800
7.5842

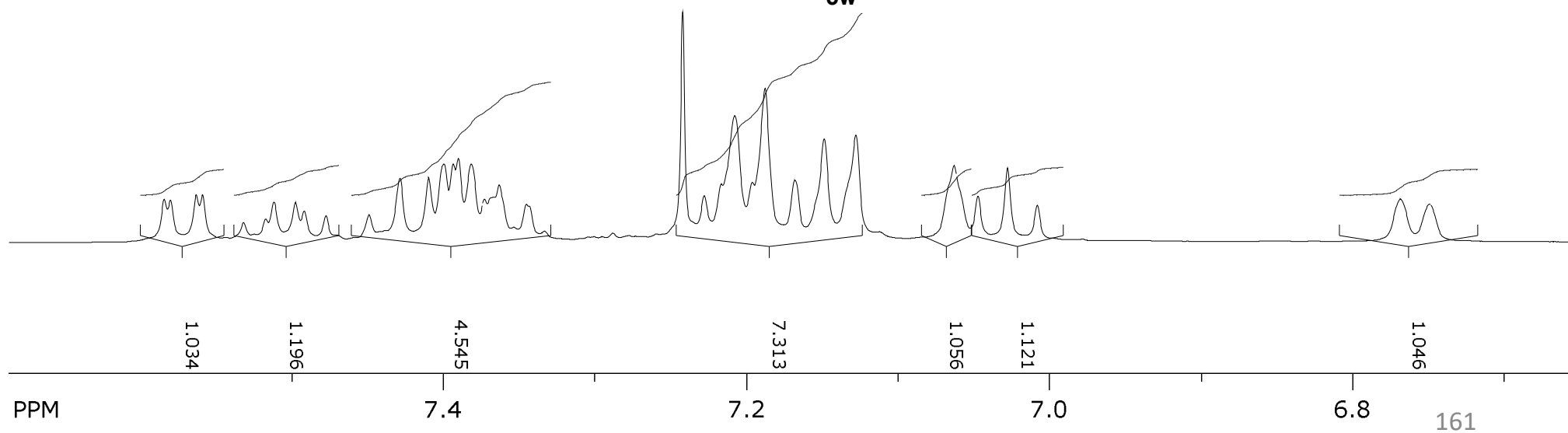
7.1276
7.1486
7.1680
7.1876
7.1961
7.2077
7.2165
7.2278
7.2419

7.0079
7.0276
7.0471
7.0628

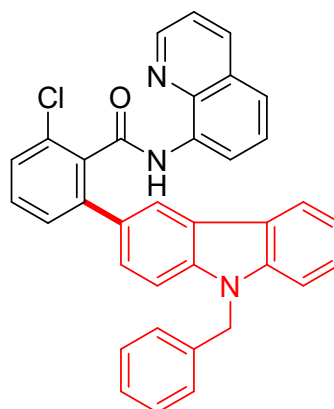
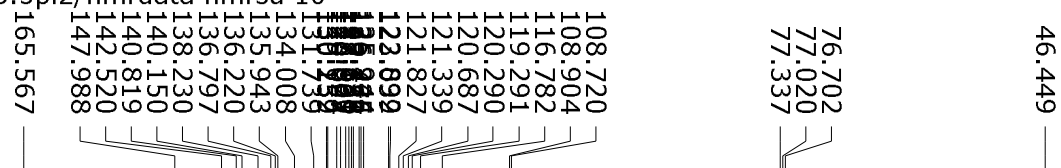
6.7490
6.7683



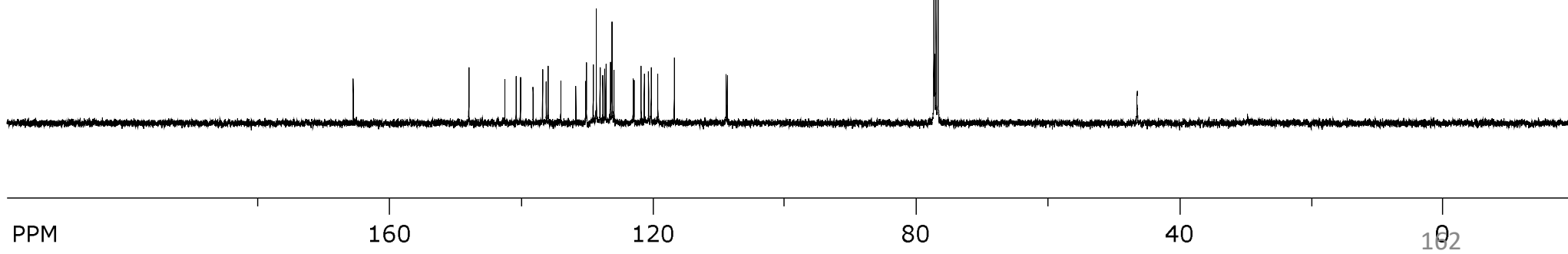
5w



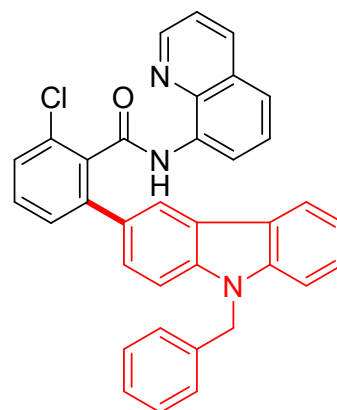
```
SpinWorks 4: RD-1273 RE1
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10
```



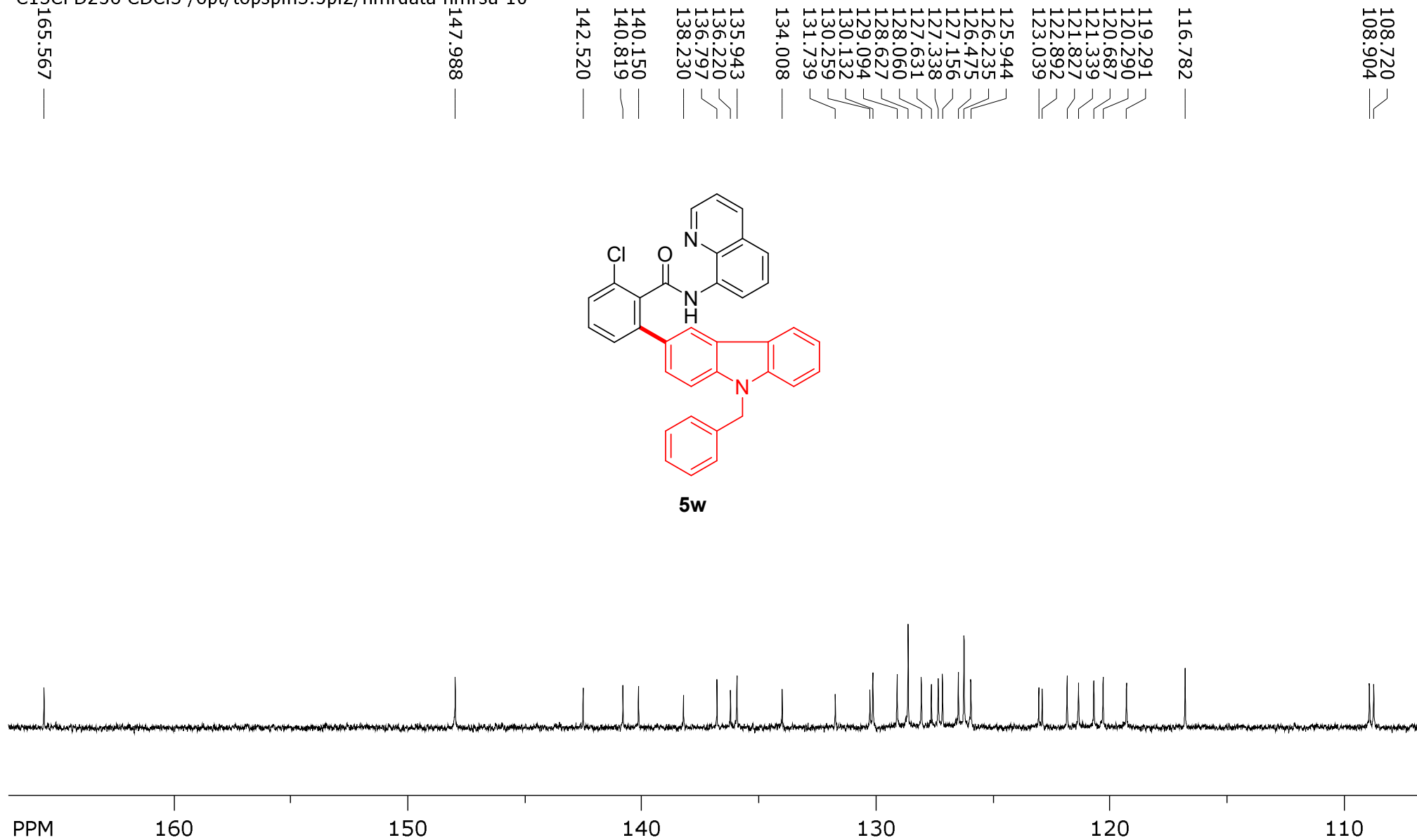
5w



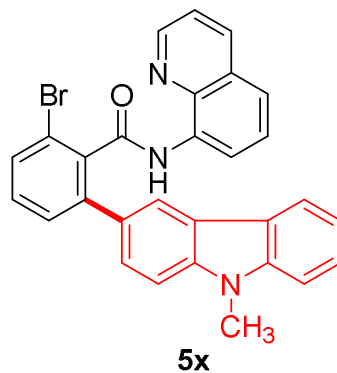
SpinWorks 4: RD-1273 RE1
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



5w



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41



SpinWorks 4: RD-1290
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

9.8044

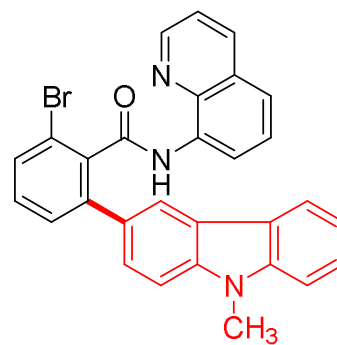
8.7221
8.7261
8.7404
8.7444

8.5517
8.5558
8.5622
8.5664

8.2480
8.2517

8.0005
8.0046
8.0212
8.0253

7.9044
7.9238



5x

1.076

1.070

1.090

1.126

1.147

PPM

9.6

9.2

8.8

8.4

8.0

SpinWorks 4: RD-1290
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

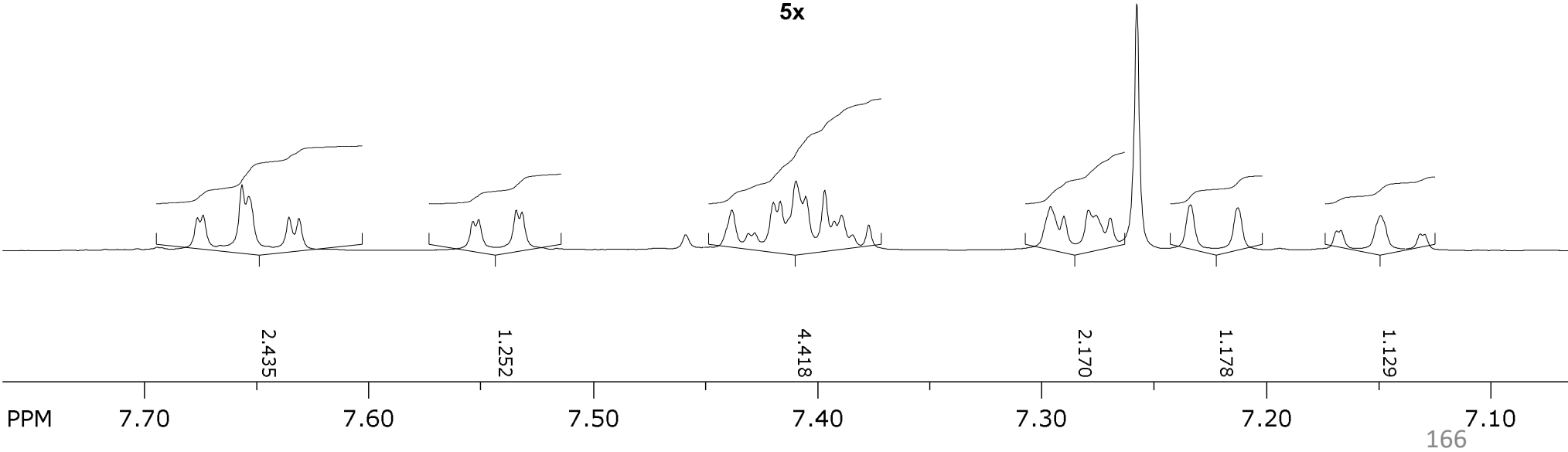
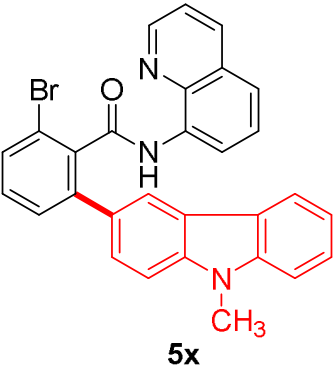
7.6313
7.6357
7.6537
7.6567
7.6740
7.6766

7.5318
7.5344
7.5512
7.5537

7.3772
7.3893
7.3926
7.3968
7.4053
7.4096
7.4166
7.4197
7.4382

7.2576
7.2695
7.2758
7.2792
7.2902
7.2961
7.2337
7.2125

7.1293
7.1312
7.1489
7.1666
7.1685

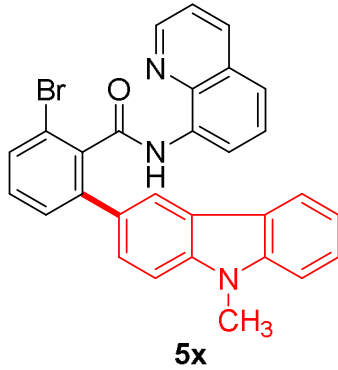


SpinWorks 4: RD-1290
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

166.458
148.063
142.812
141.208
140.480
138.348
138.337
136.024
134.120
131.235
130.380
129.580
129.578
129.576
129.574
121.379
120.654
120.584
120.260
118.945
116.839
108.420
108.277

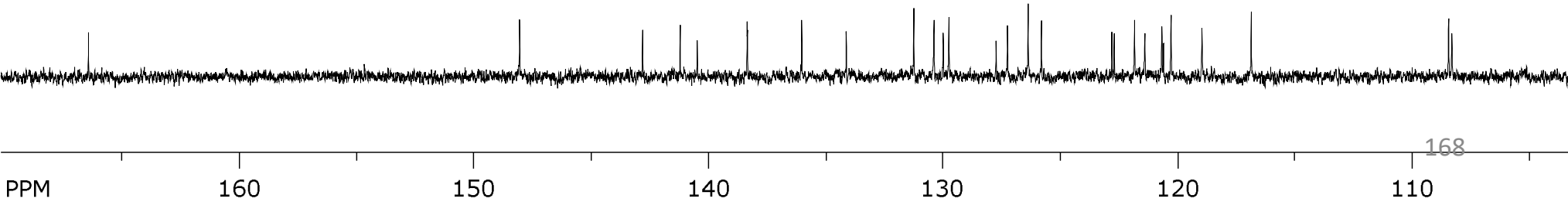
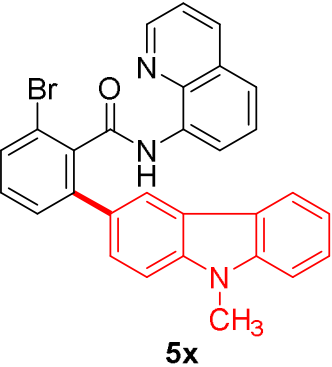
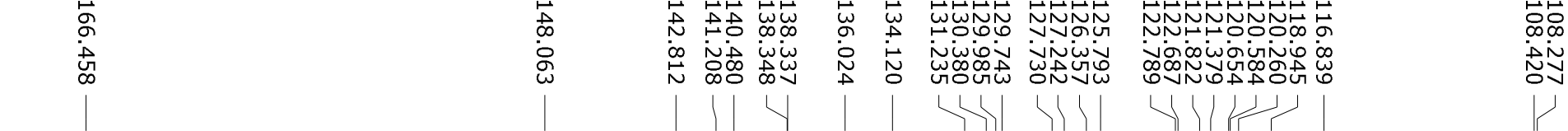
76.702
77.020
77.337

28.973

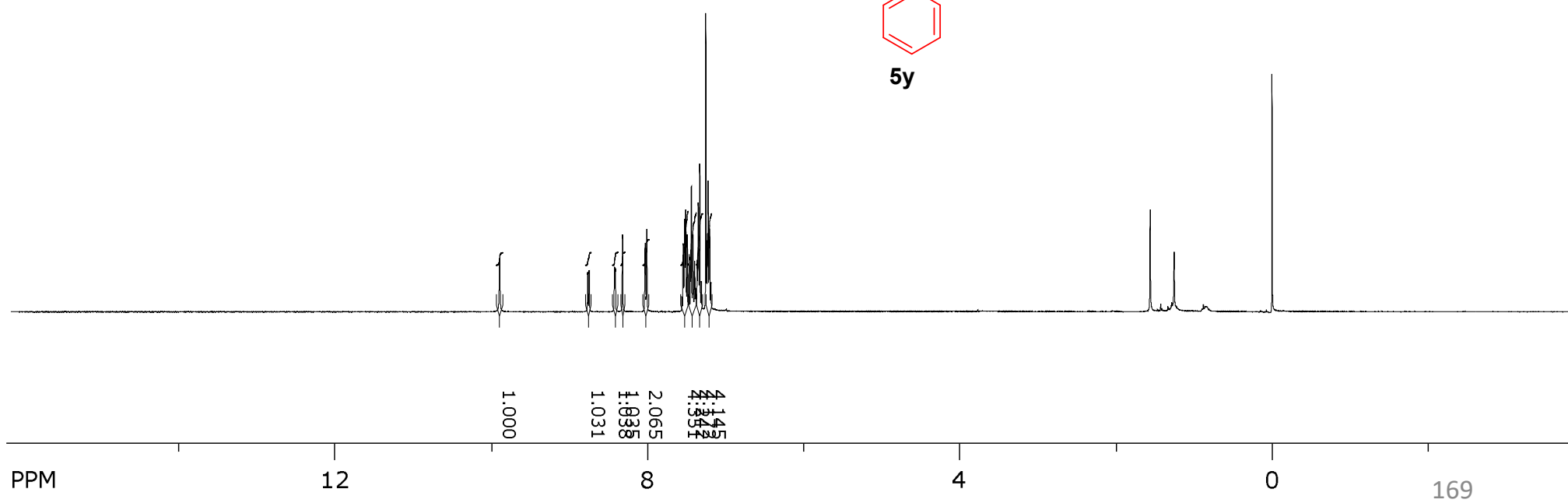
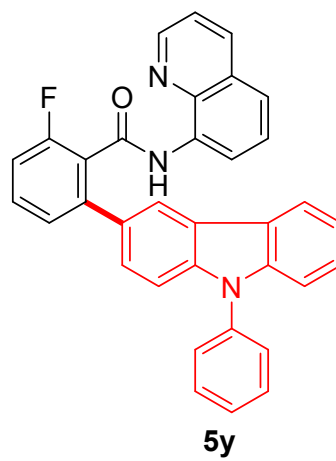
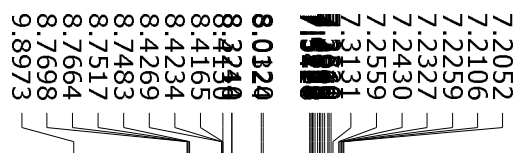


PPM 160 120 80 40 0

SpinWorks 4: RD-1290
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5



SpinWorks 4: RD-893
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

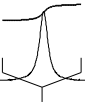
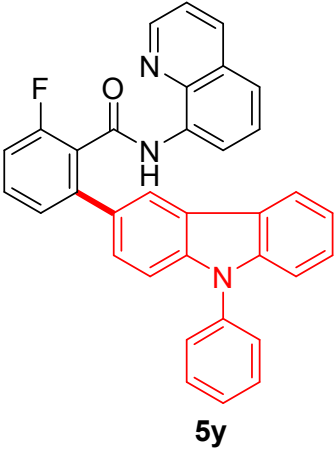
9.8973

8.7483
8.7517
8.7664
8.7698

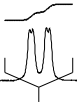
8.4130
8.4165
8.4234
8.4269

8.3210
8.3244

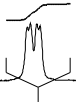
8.0120
8.0324



1.000



1.031



1.038



1.035



2.065

PPM

9.6

9.2

8.8

8.4

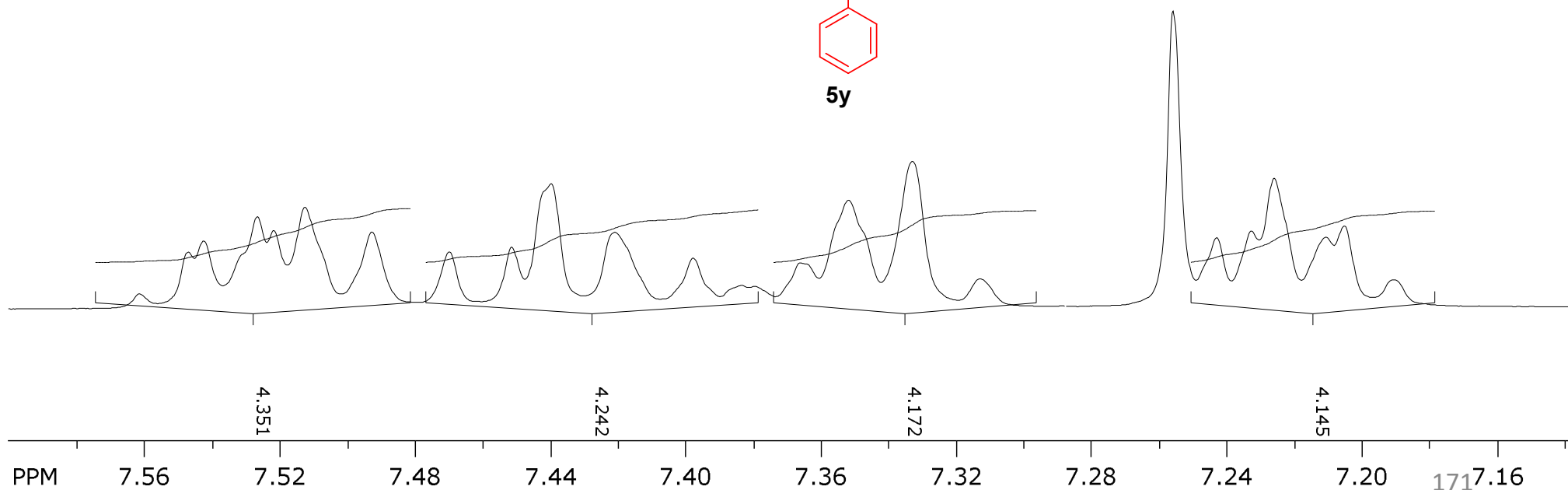
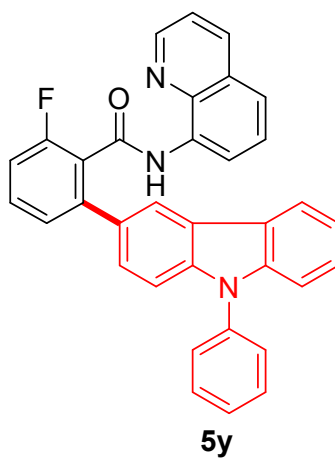
170

8.0

SpinWorks 4: RD-893

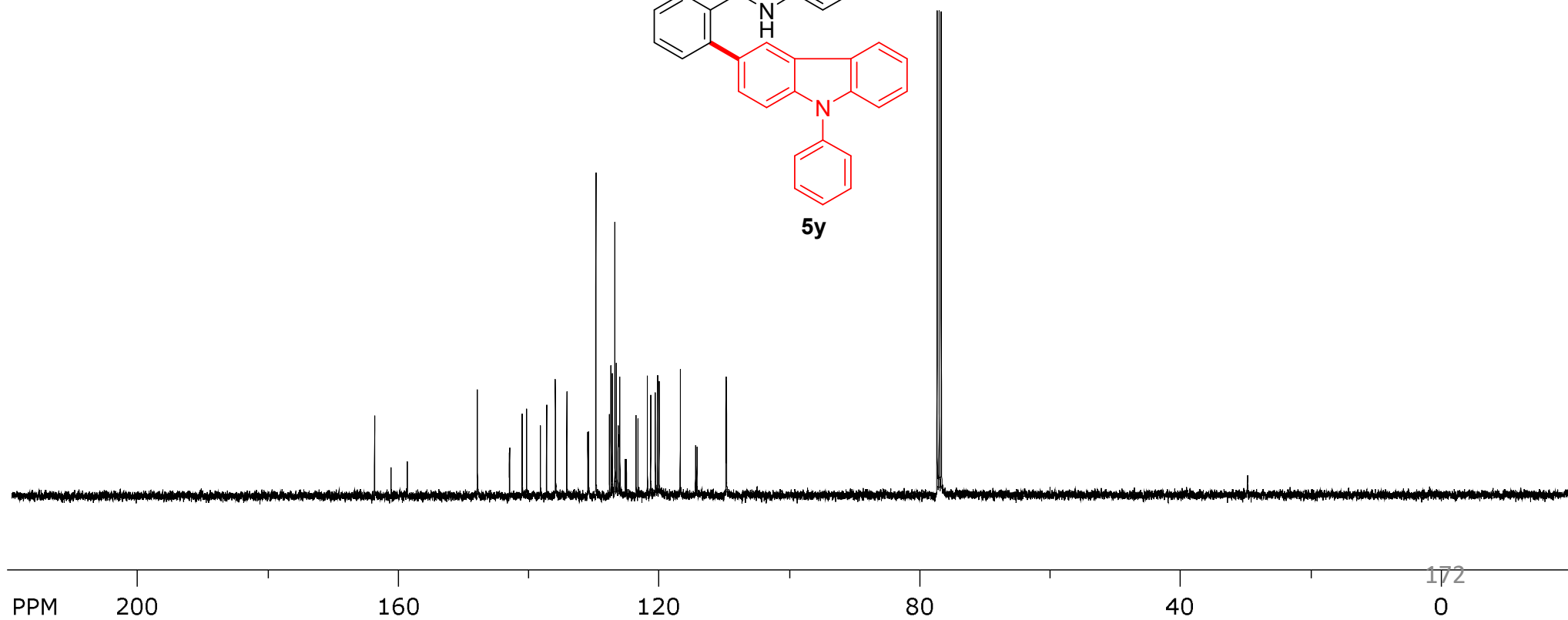
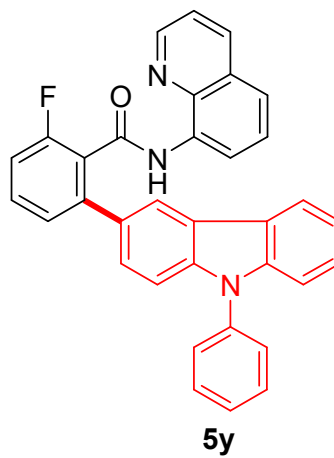
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

7.2052 —
7.2106 —
7.2259 —
7.2327 —
7.2430 —
7.2559 —
7.3131 —
7.3330 —
7.3519 —
7.3661 —
7.3979 —
7.4211 —
7.4399 —
7.4516 —
7.4700 —
7.4930 —
7.5128 —
7.5220 —
7.5269 —
7.5428 —
7.5474 —

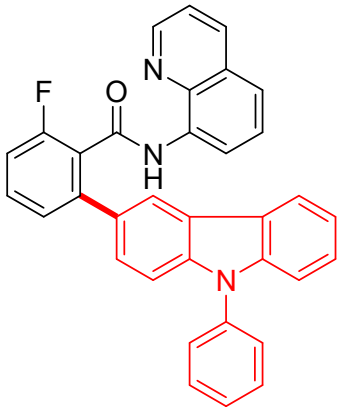


C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

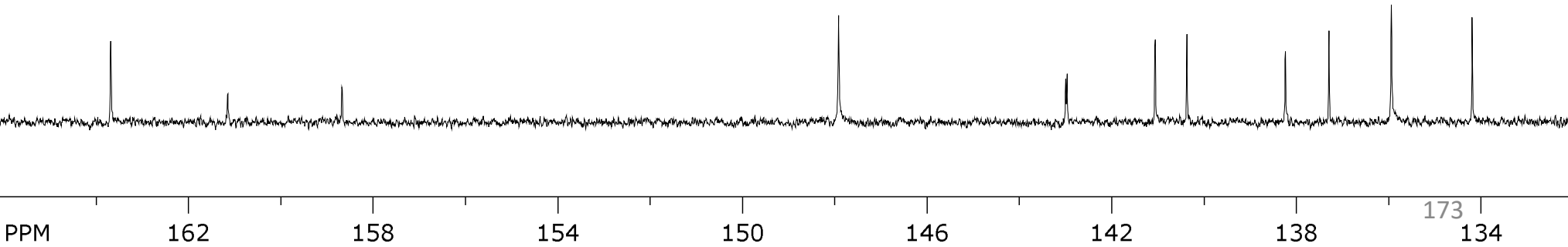
76.703	109.677
77.020	109.741
77.338	114.198
	114.417
	116.771
	120.022
	120.260
	120.589
	121.805
	121.955
	121.955
	130.944
	130.944
	134.181
	135.931
	137.285
	138.231
	140.364
	141.053
	142.961
	147.996
	147.996
	158.677
	161.155
	163.690



SpinWorks 4: RD-893
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

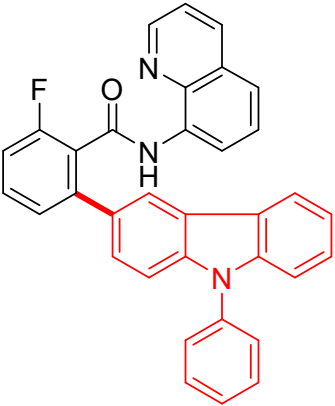


5y

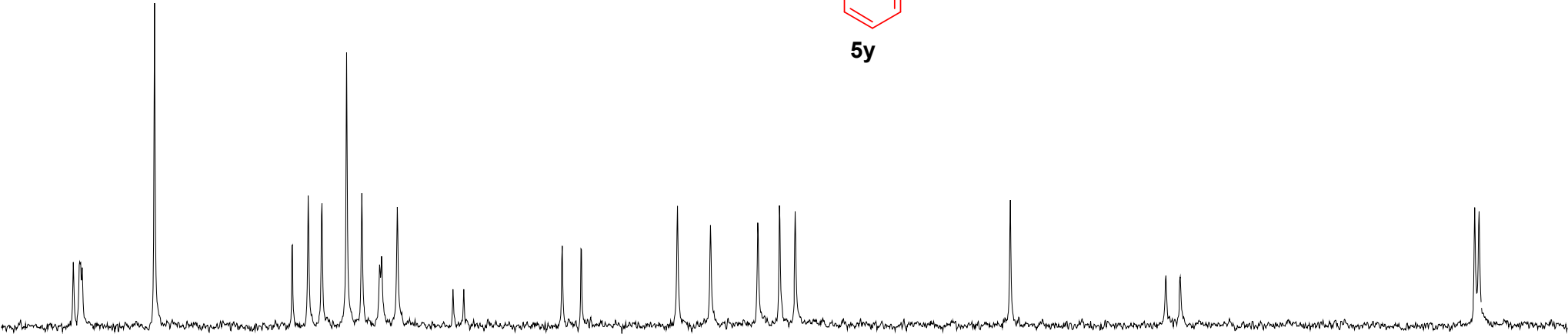


SpinWorks 4: RD-893
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

130.813
130.838
130.848
130.944
129.720
127.637
127.392
127.184
126.810
126.584
126.312
126.284
126.044
125.205
125.038
123.552
123.263
121.809
121.305
120.589
120.260
120.022
116.771
114.417
114.198
109.741
109.677

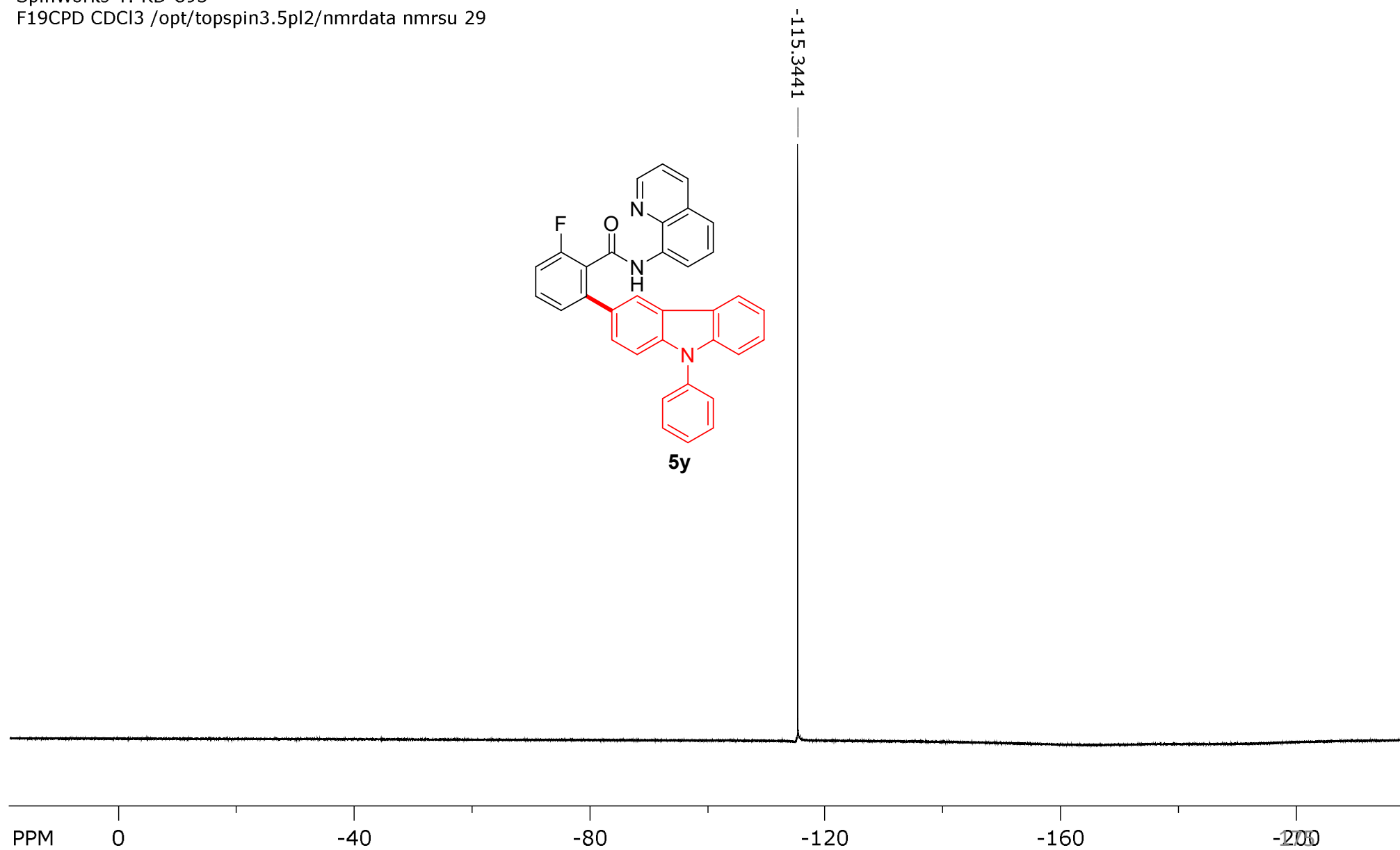
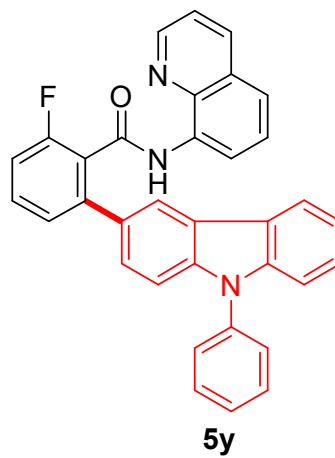


5y



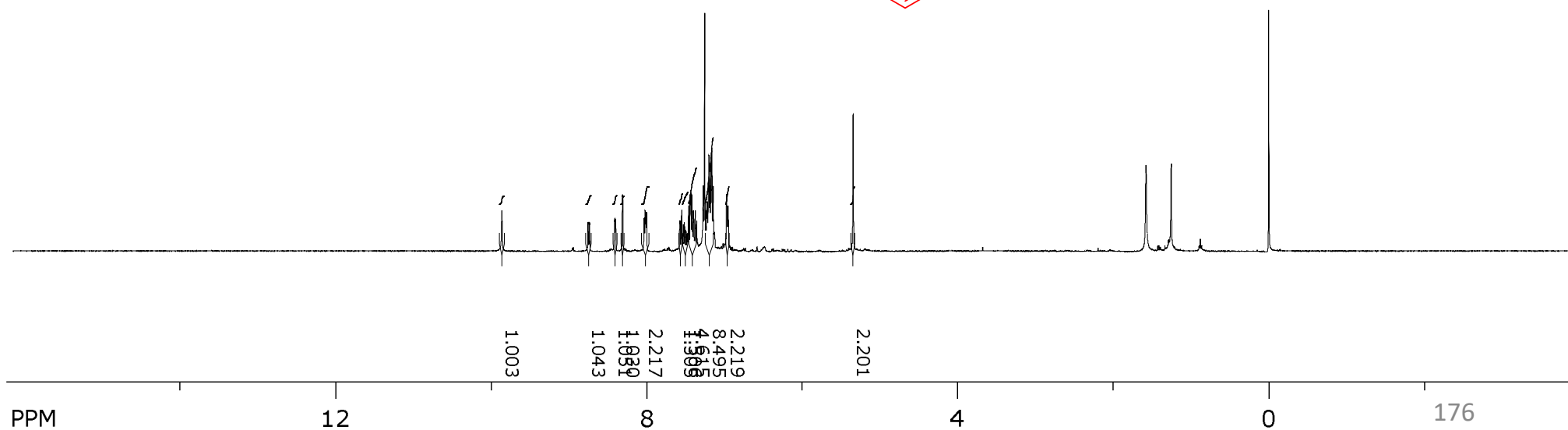
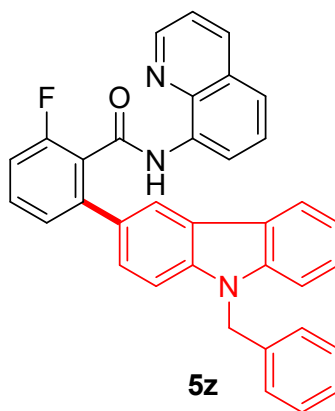
PPM 128 124 120 116 112 174

SpinWorks 4: RD-893
F19CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29



SpinWorks 4: RD-889

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: RD-889

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

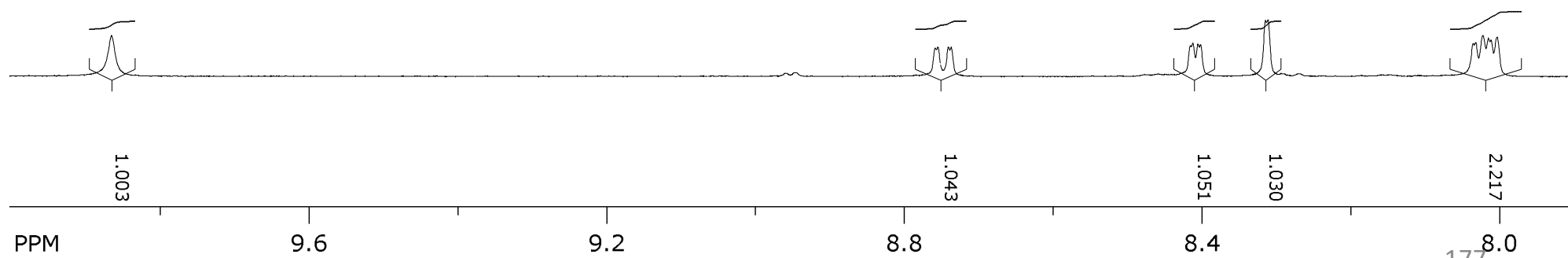
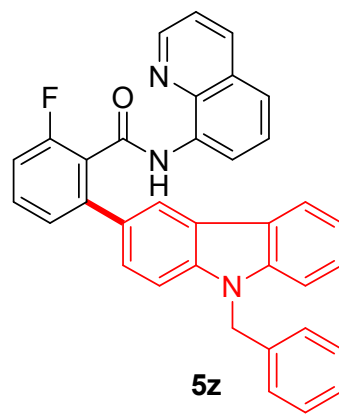
9.8656

8.7370
8.7408
8.7549
8.7586

8.4019
8.4053
8.4122
8.4156

8.3113
8.3145

8.0032
8.0113
8.0149
8.0223
8.0320
8.0353

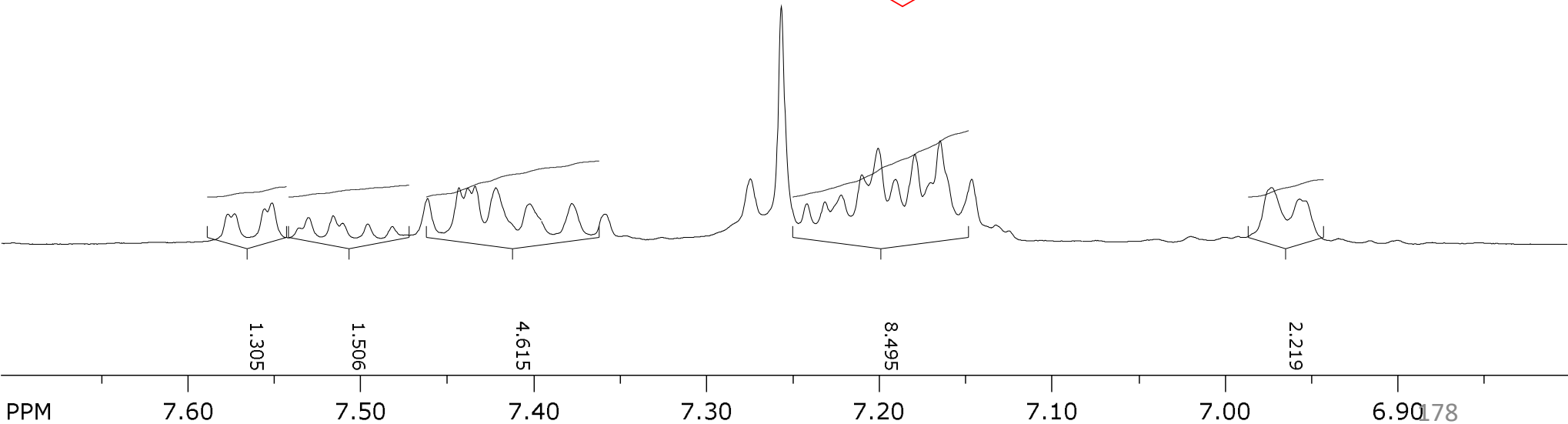
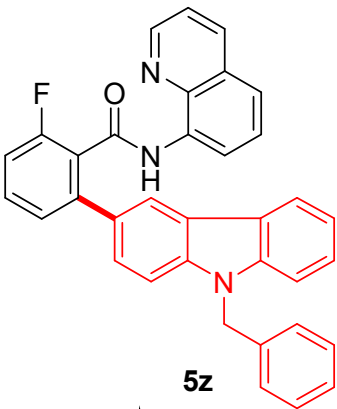


SpinWorks 4: RD-889
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

7.3586
7.3780
7.4025
7.4220
7.4340
7.4382
7.4433
7.4617
7.4825
7.4960
7.5162
7.5305
7.5517
7.5559
7.5732
7.5771

7.2747
7.2568
7.2420
7.2315
7.2221
7.2101
7.2006
7.1907
7.1794
7.1703
7.1649
7.1465

6.9537
6.9568
6.9730

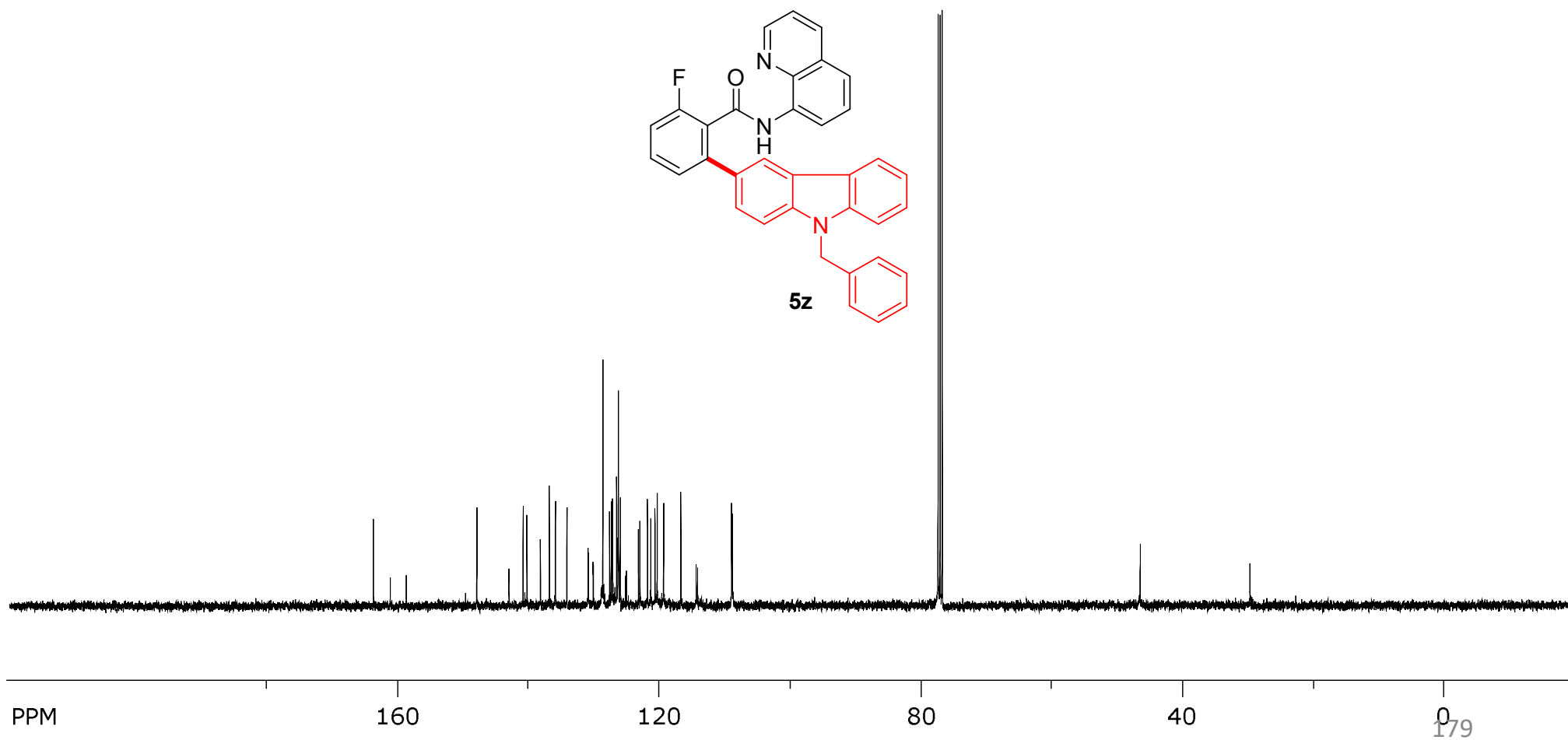
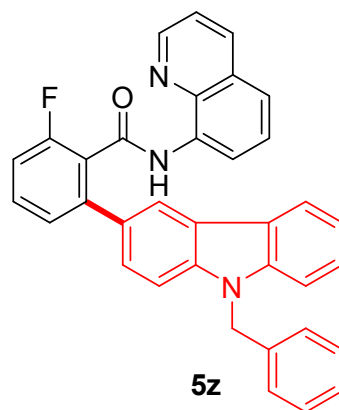


C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

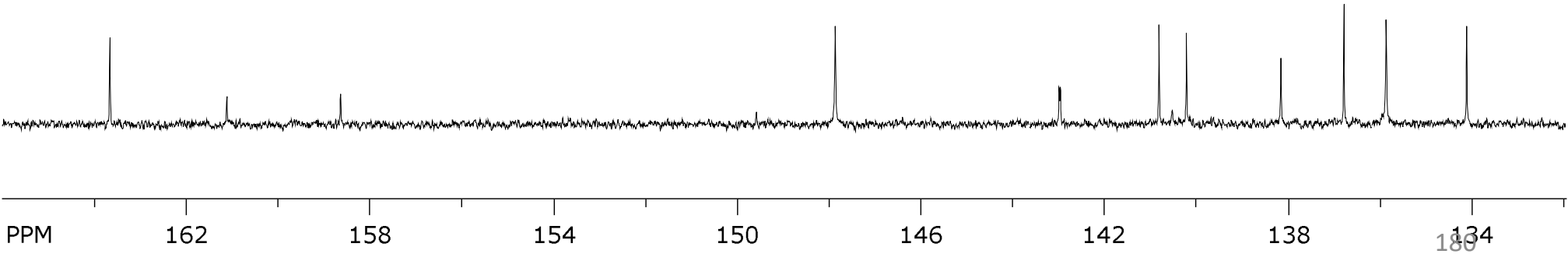
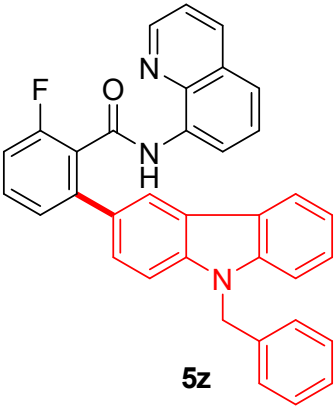
108.781	131.329
108.914	130.900
114.102	130.000
114.322	130.000
116.666	130.000
119.312	130.000
120.294	120.631
120.631	134.099
134.099	135.856
135.856	136.775
136.775	138.148
140.208	140.807
142.955	142.955
142.955	147.983
147.983	158.650
158.650	161.129
161.129	163.680
163.680	

76.702
77.020
77.337

46.430

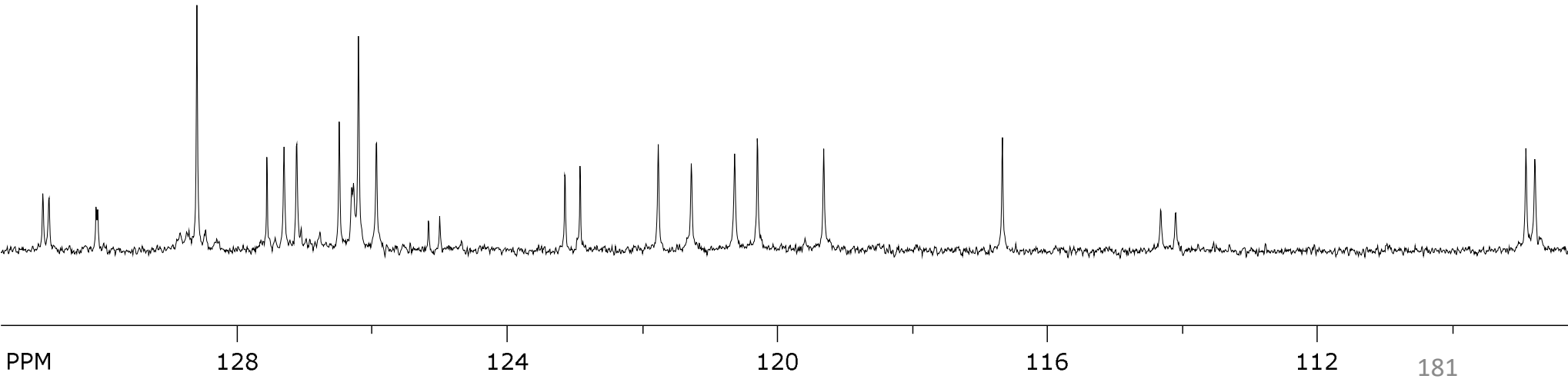
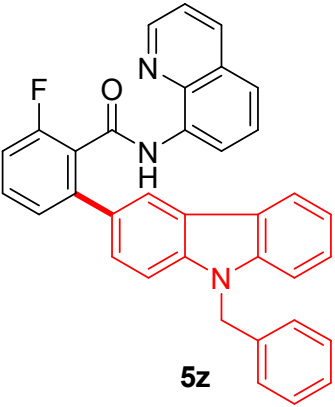
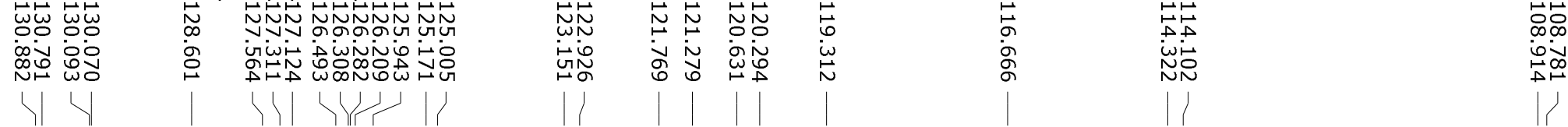


SpinWorks 4: RD 889
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

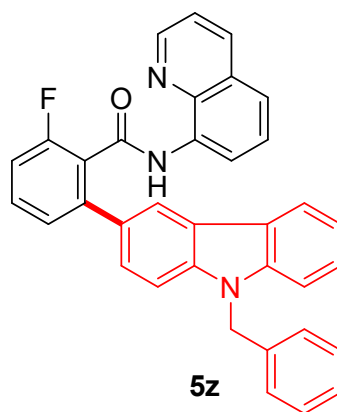


SpinWorks 4: RD 889

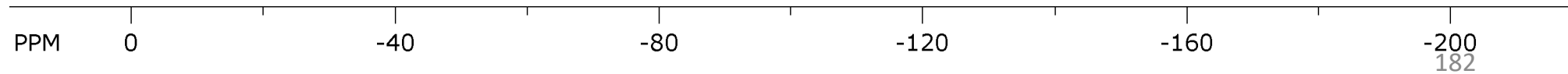
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



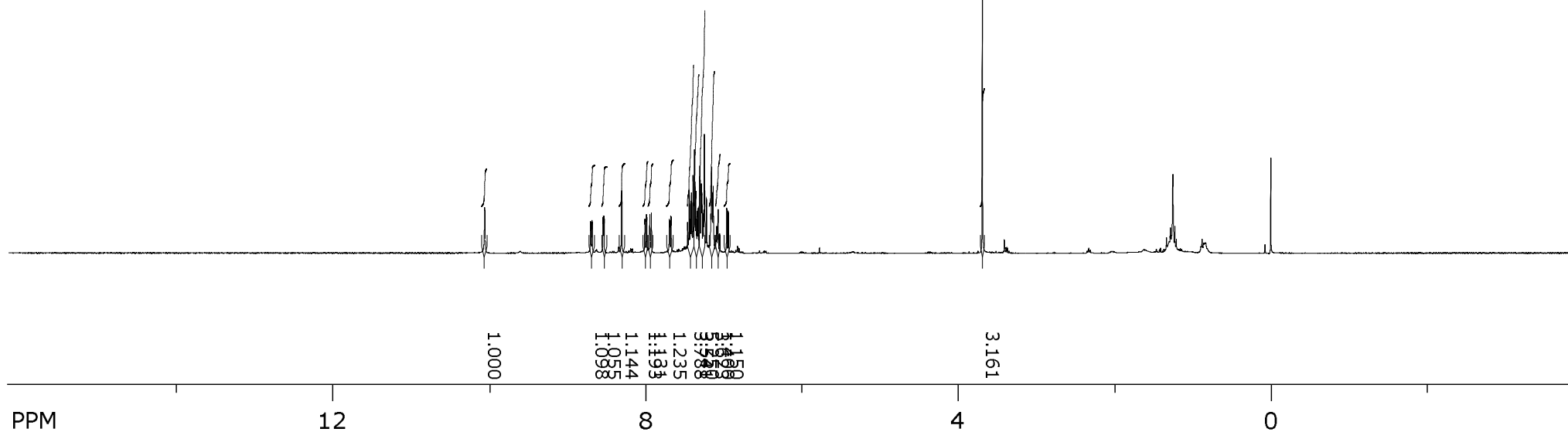
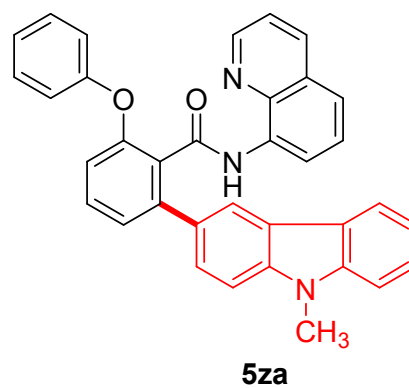
SpinWorks 4: RD-889
F19CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 44



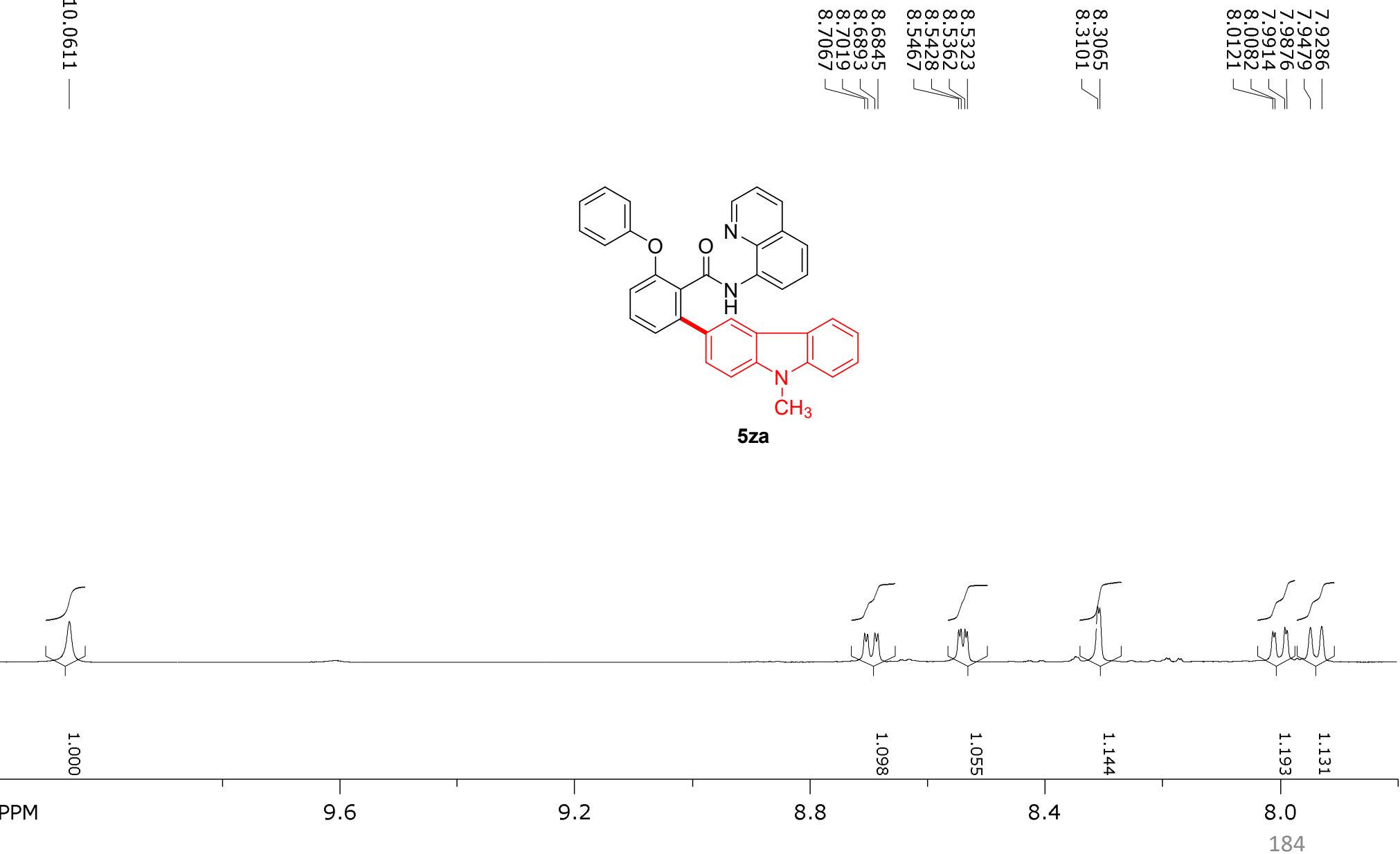
-115.3906



PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56

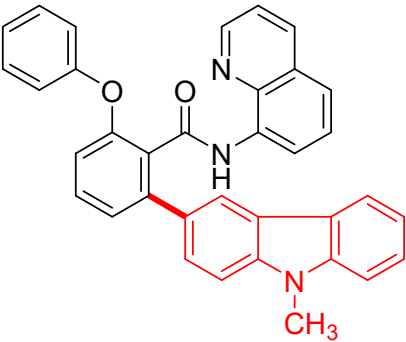


SpinWorks 4: RD-765
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56

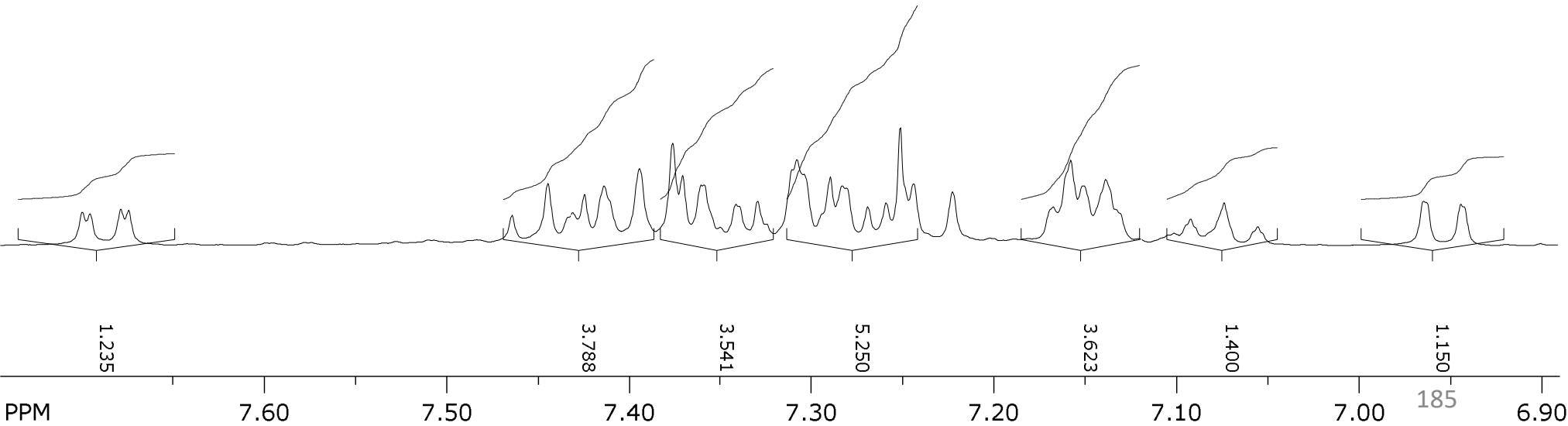


SpinWorks 4: RD-765
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 56

7.6744	7.4642	7.2227	7.1387	7.0554	6.9425
7.6787	7.4446	7.2441	7.1511	7.0738	6.9645
7.6956	7.4309	7.2514	7.1580	7.0922	
7.6998	7.4245	7.2692	7.1676		
	7.4137	7.2809			
	7.3943	7.2832			
	7.3762	7.2897			
	7.3707	7.3042			
	7.3606	7.3081			
	7.3589	7.3107			
	7.3501	7.3248			
	7.3415	7.3296			
	7.3296	7.3248			
	7.3107	7.3042			
	7.3081	7.2897			
	7.3042	7.2832			
	7.2897	7.2809			
	7.2832	7.2692			
	7.2692	7.2514			
	7.2514	7.2441			
	7.2441	7.2227			

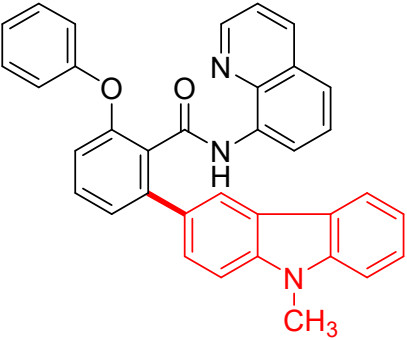


5za



SpinWorks 4: RD-765
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38

108.244
108.359
116.665
118.833
119.559
120.222
120.513
121.240
121.456
121.866
122.156
122.404
122.804
123.004
129.084
130.263
130.478
130.478
134.440
135.924
138.317
140.373
141.162
142.972
147.864
154.845
156.960
165.620
76.702
77.020
77.337
28.899

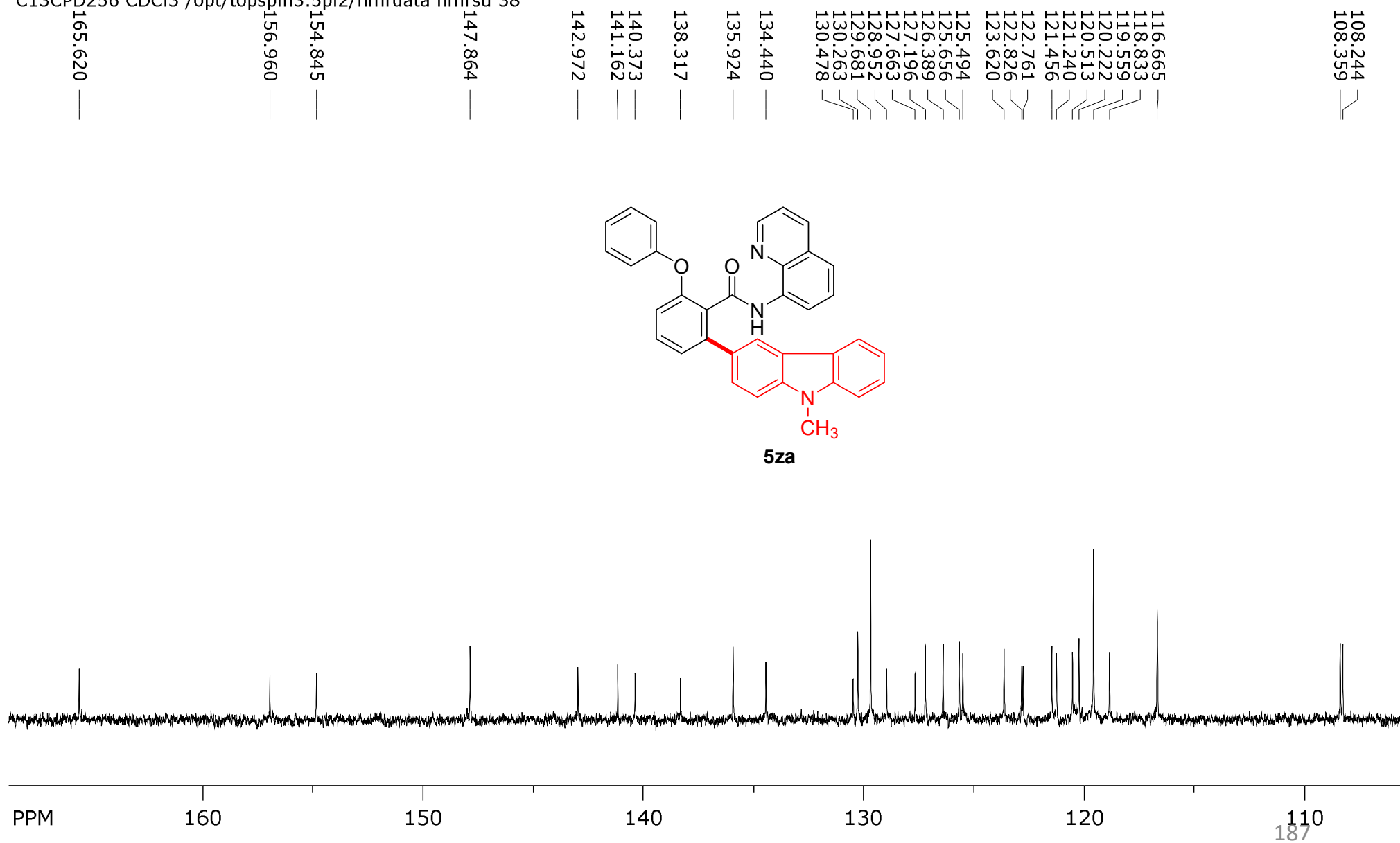


5za

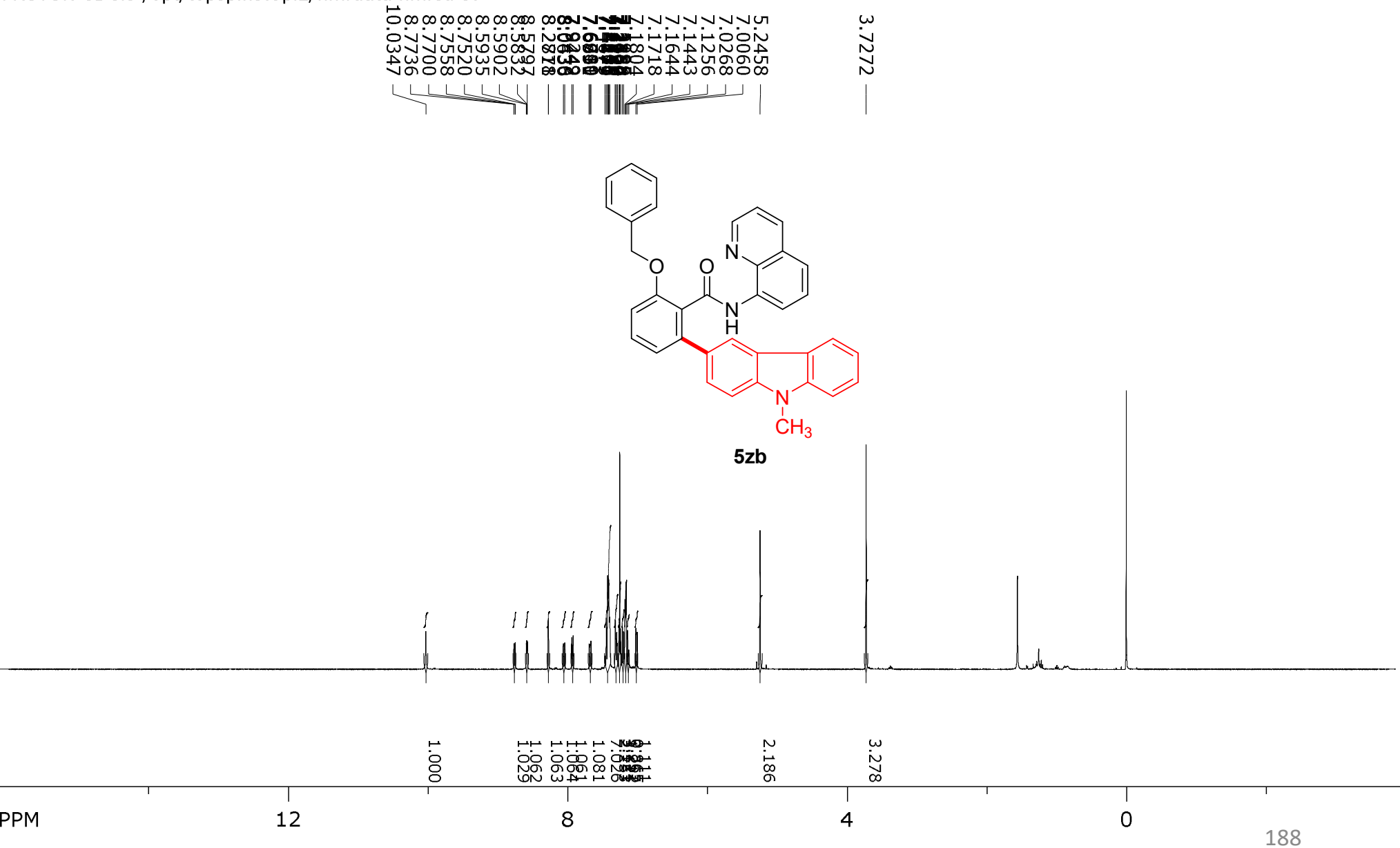
PPM 160 120 80 40 0 186

SpinWorks 4: RD-765

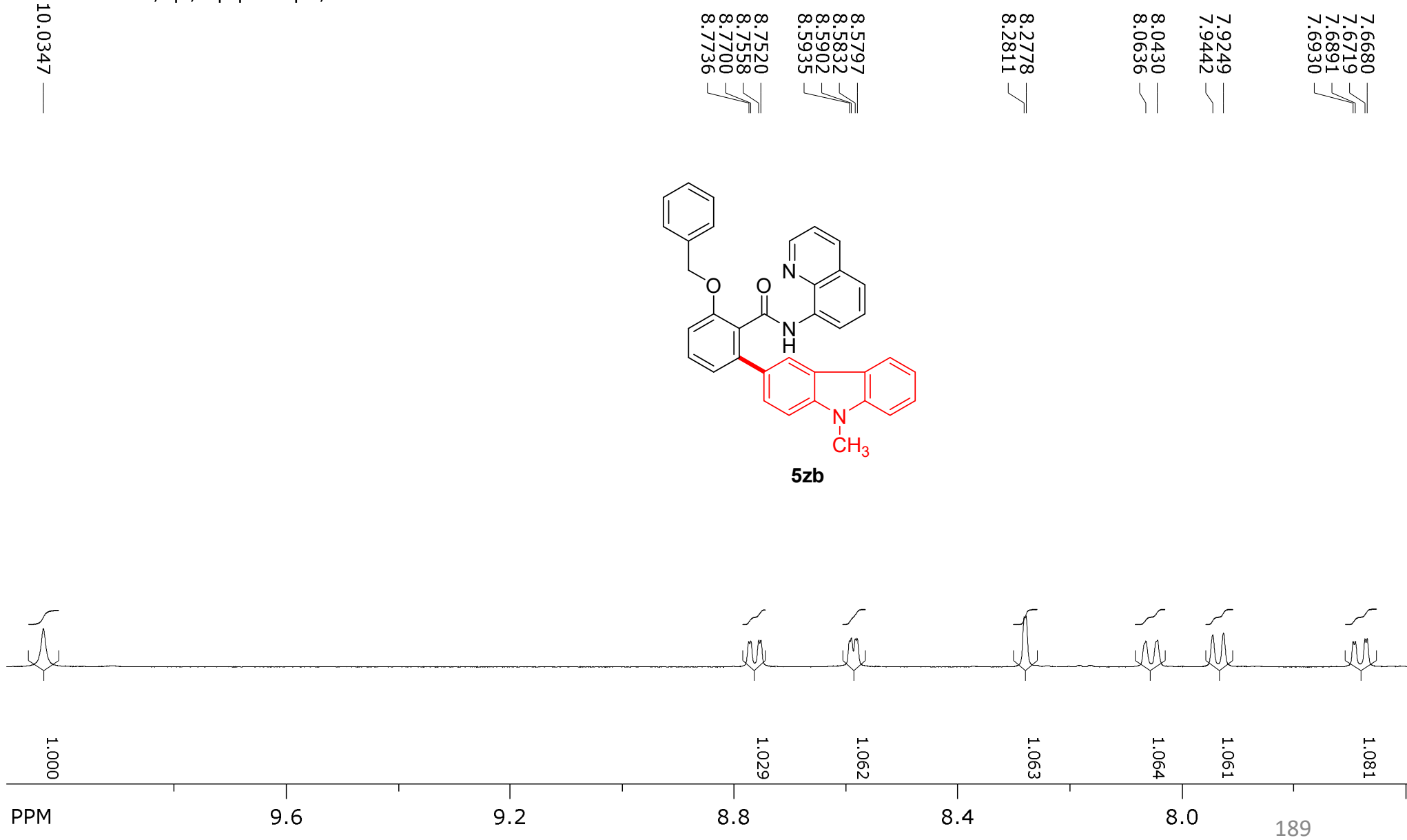
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38



SpinWorks 4: RD 916
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 37



PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 37



SpinWorks 4: RD 916

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 37

7.6680
7.6719
7.6891
7.6930

7.4011
7.4111
7.4168
7.4220
7.4295
7.4479
7.4673

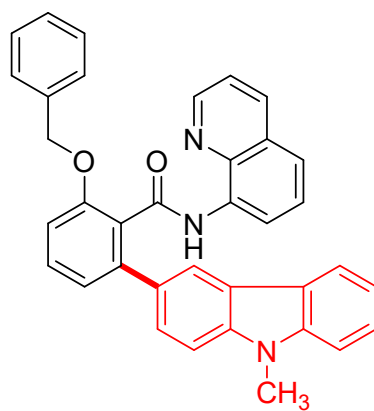
7.2926
7.2996
7.3136
7.3195

7.2456
7.2564
7.2667

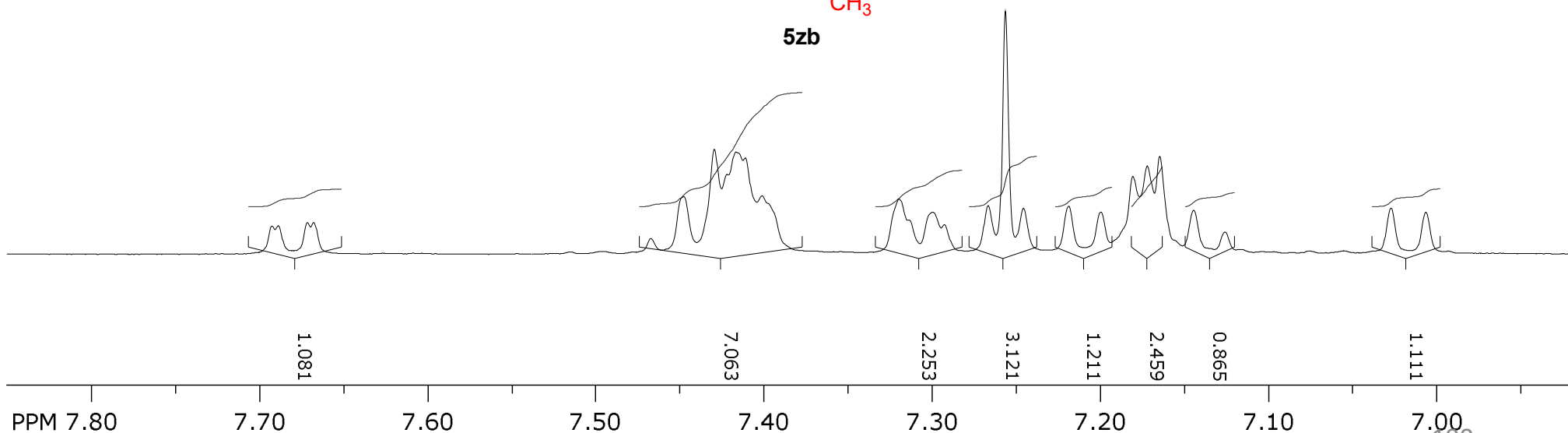
7.1256
7.1443
7.1644
7.1718
7.1804

7.1995
7.2188

7.0060
7.0268



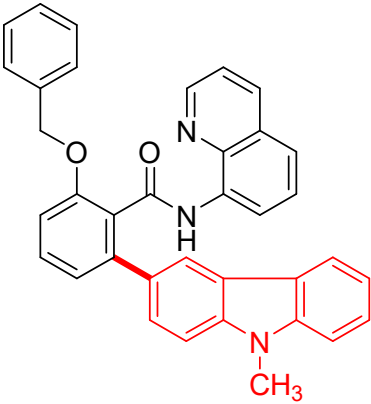
5zb



SpinWorks 4: RD 916
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 37

5.2458

3.7272



5zb

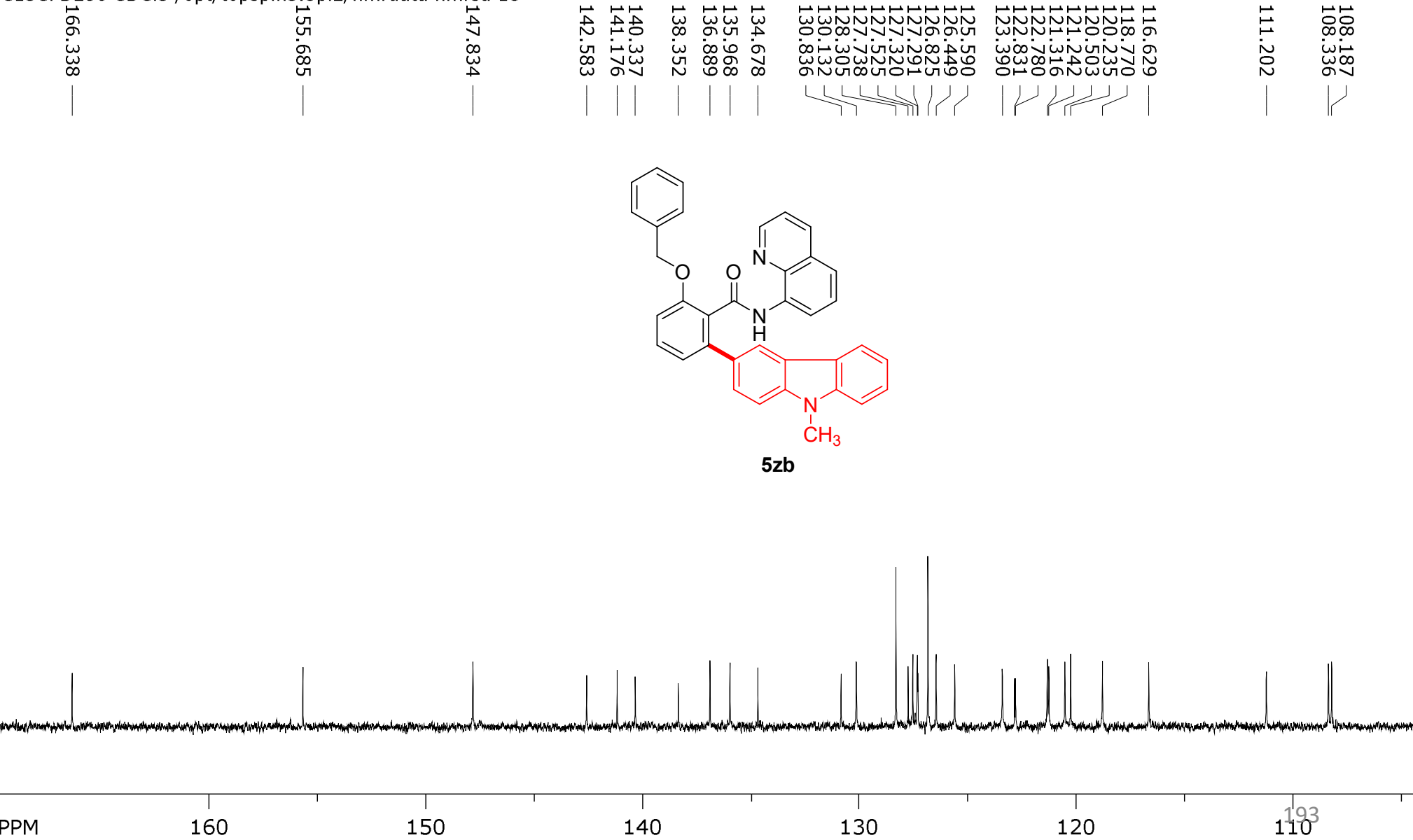
2.186

3.278

PPM 5.6 5.2 4.8 4.4 4.0 3.6 3.2

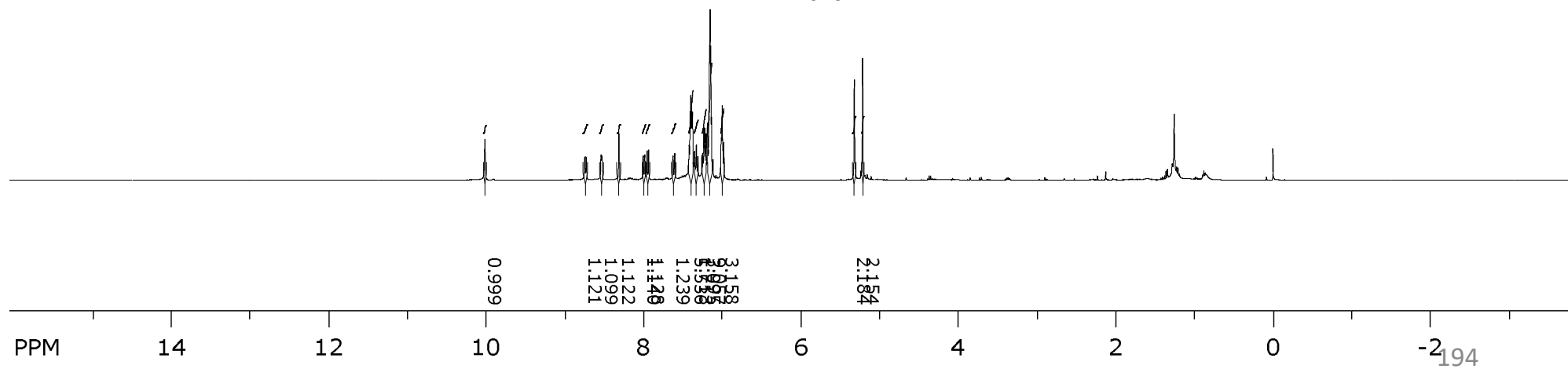
191

SpinWorks 4: RD 916
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

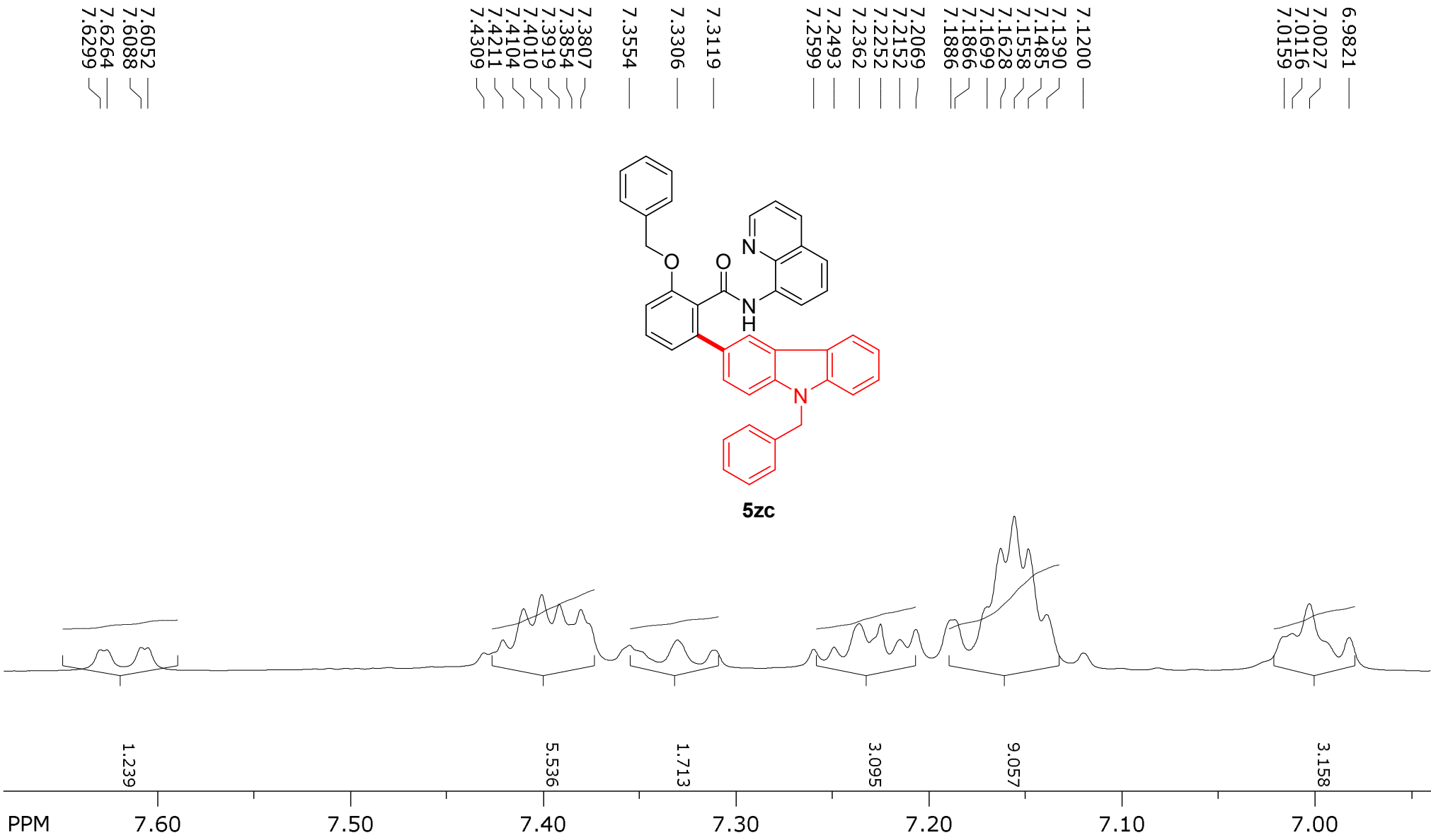
5	2.169
5	3.223
6	.9821
7	.0027
7	.0116
7	.0159
7	.1200
7	.1390
7	.1485
7	.1500
7	.6059
7	.9383
7	.9576
7	.9855
8	.0060
8	.3159
8	.5339
8	.5412
8	.7314
8	.7489
10	.0191



SpinWorks 4: RD-919 RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



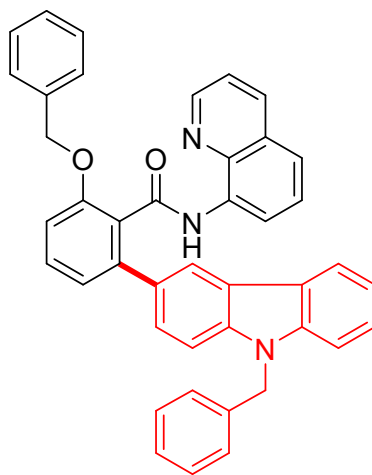
SpinWorks 4: RD-919 RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



SpinWorks 4: RD-919 RE
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

5.3223

5.2169



5zc

2.184

2.154

PPM

5.50

5.40

5.30

5.20

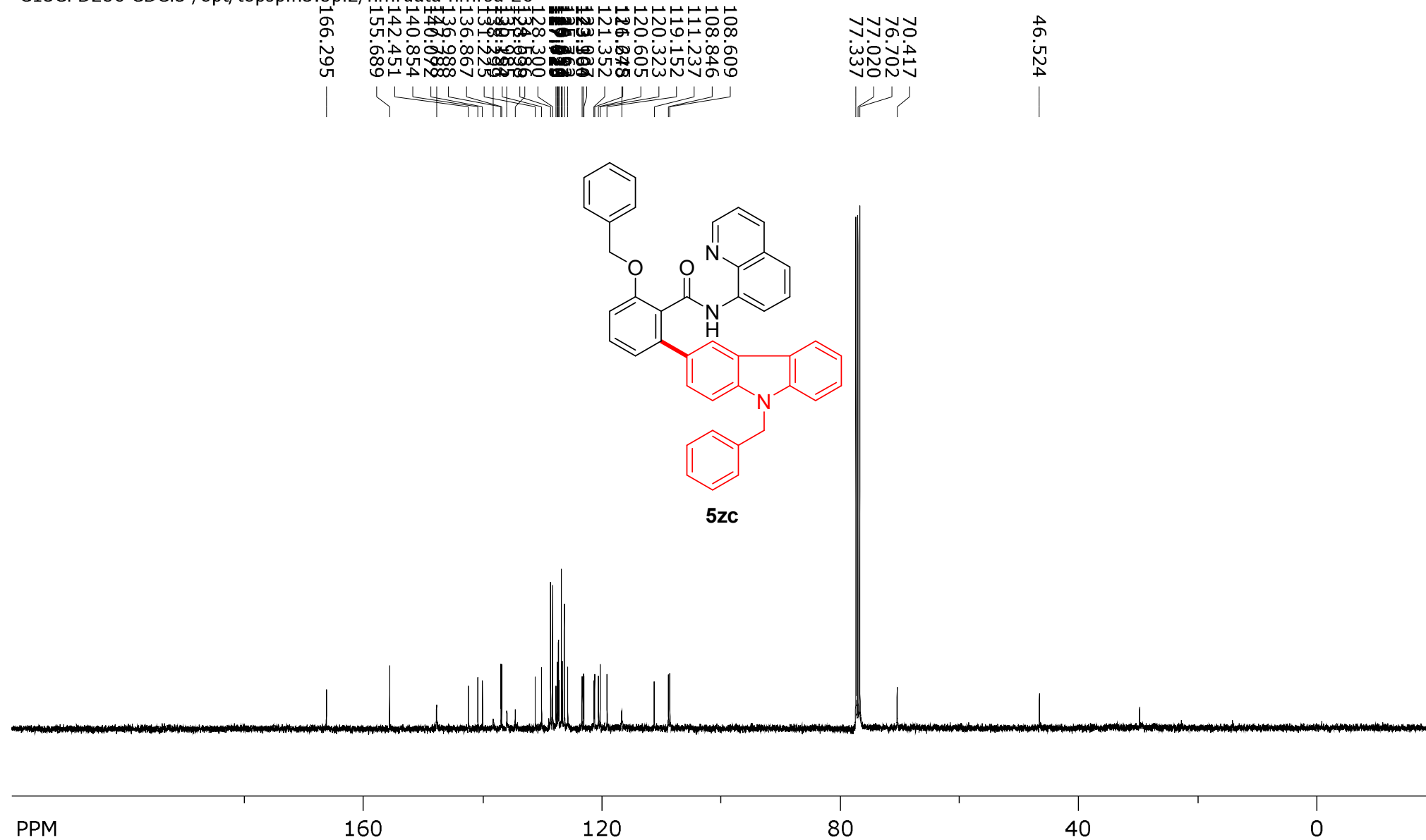
5.10

5.00

197

SpinWorks 4: RD-919 RE

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



SpinWorks 4: RD-919 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

166.295

155.689

147.788

142.451

140.854

140.072

138.299

136.867

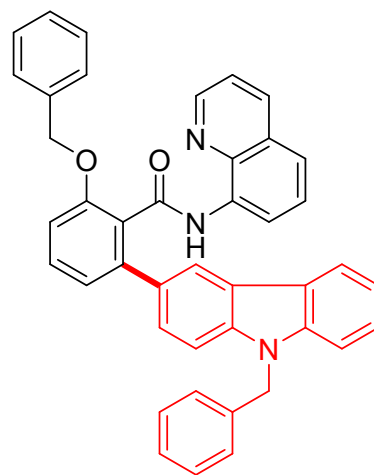
136.988

135.985

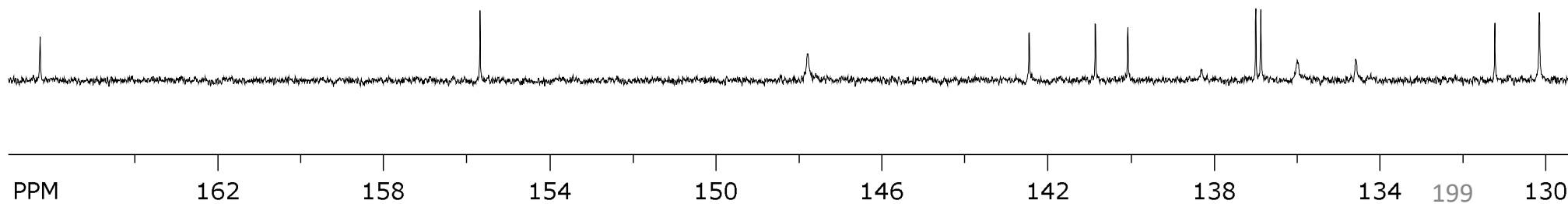
134.586

131.225

130.154

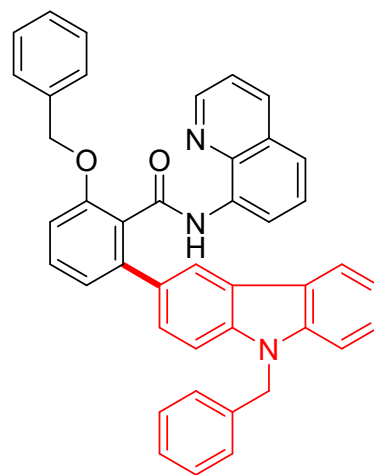


5zc

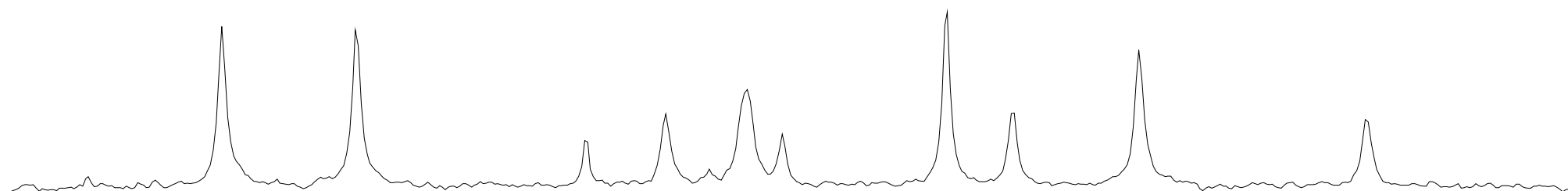


SpinWorks 4: RD-919 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

128.638 —
128.300 —
127.723 —
127.523 —
127.415 —
127.320 —
127.230 —
126.817 —
126.651 —
126.333 —
125.762 —



5zc



PPM

128.8

128.4

128.0

127.6

127.2

126.8

126.4

126.0

125.6

200

SpinWorks 4: RD-919 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

123.037
123.104
123.360

121.245
121.352

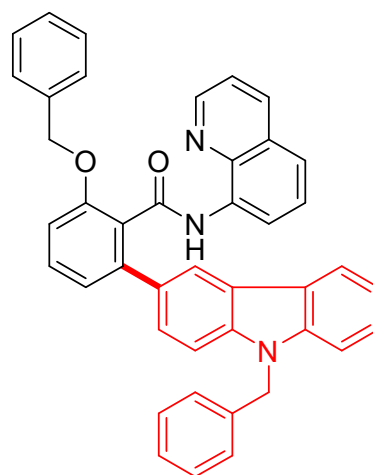
120.323
120.605

119.152

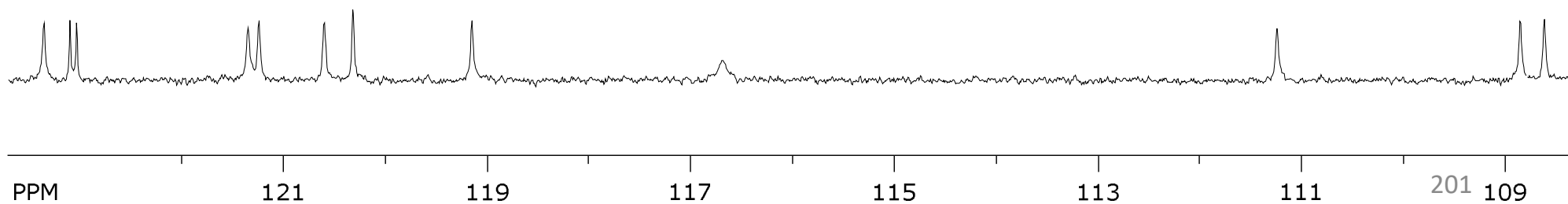
116.678

111.237

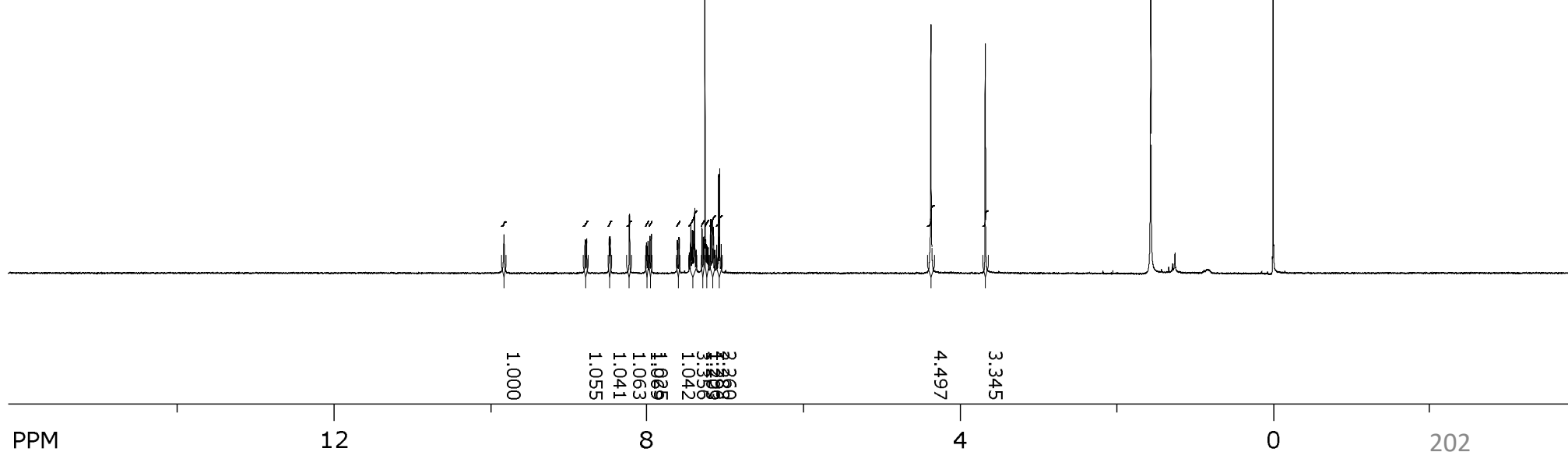
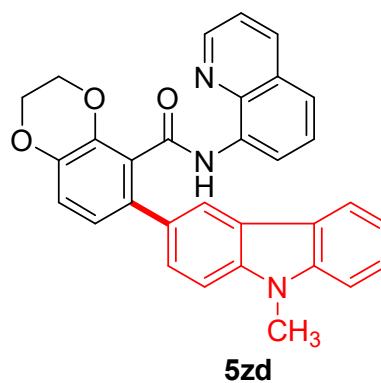
108.609
108.846



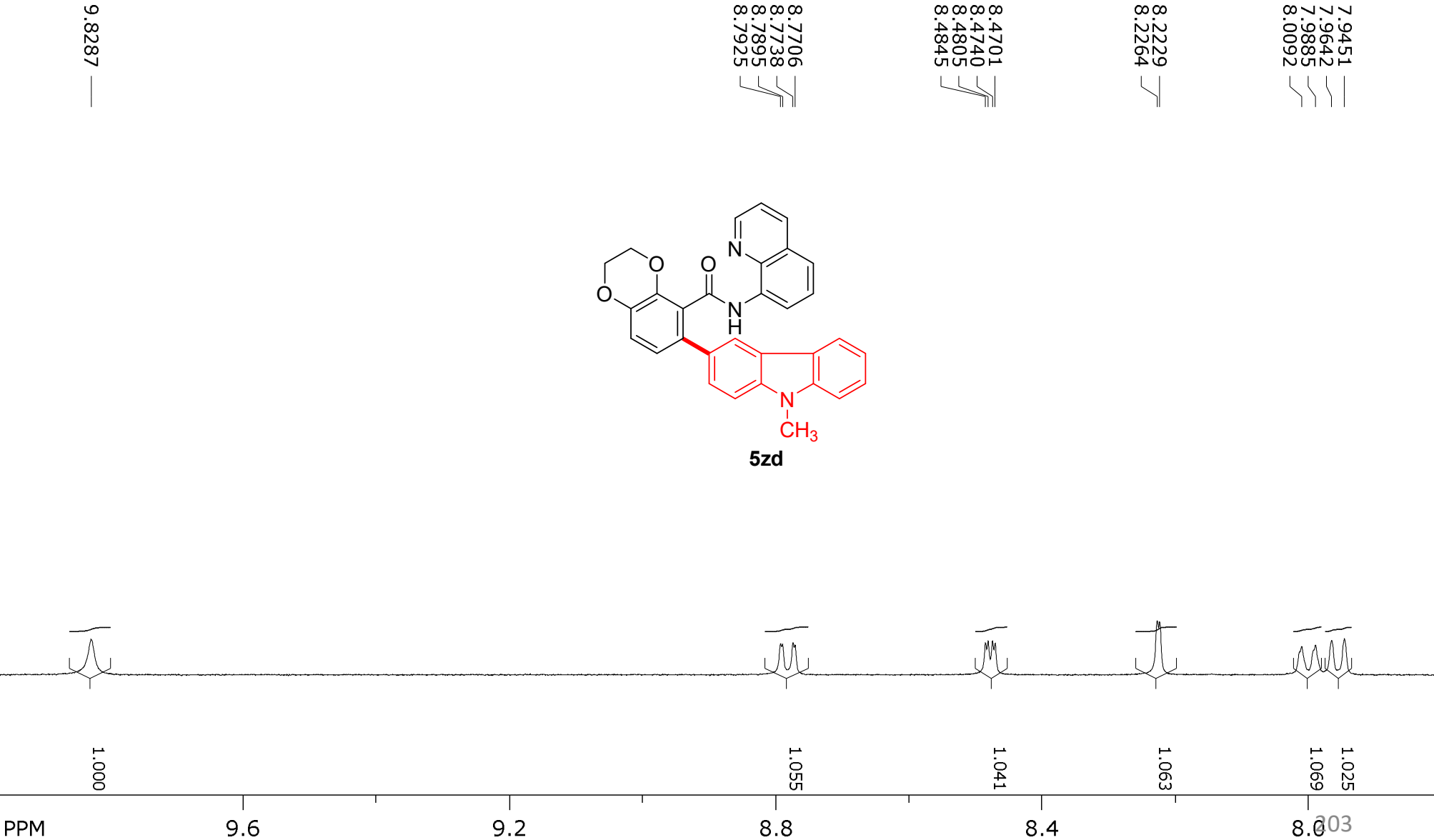
5zc



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 55

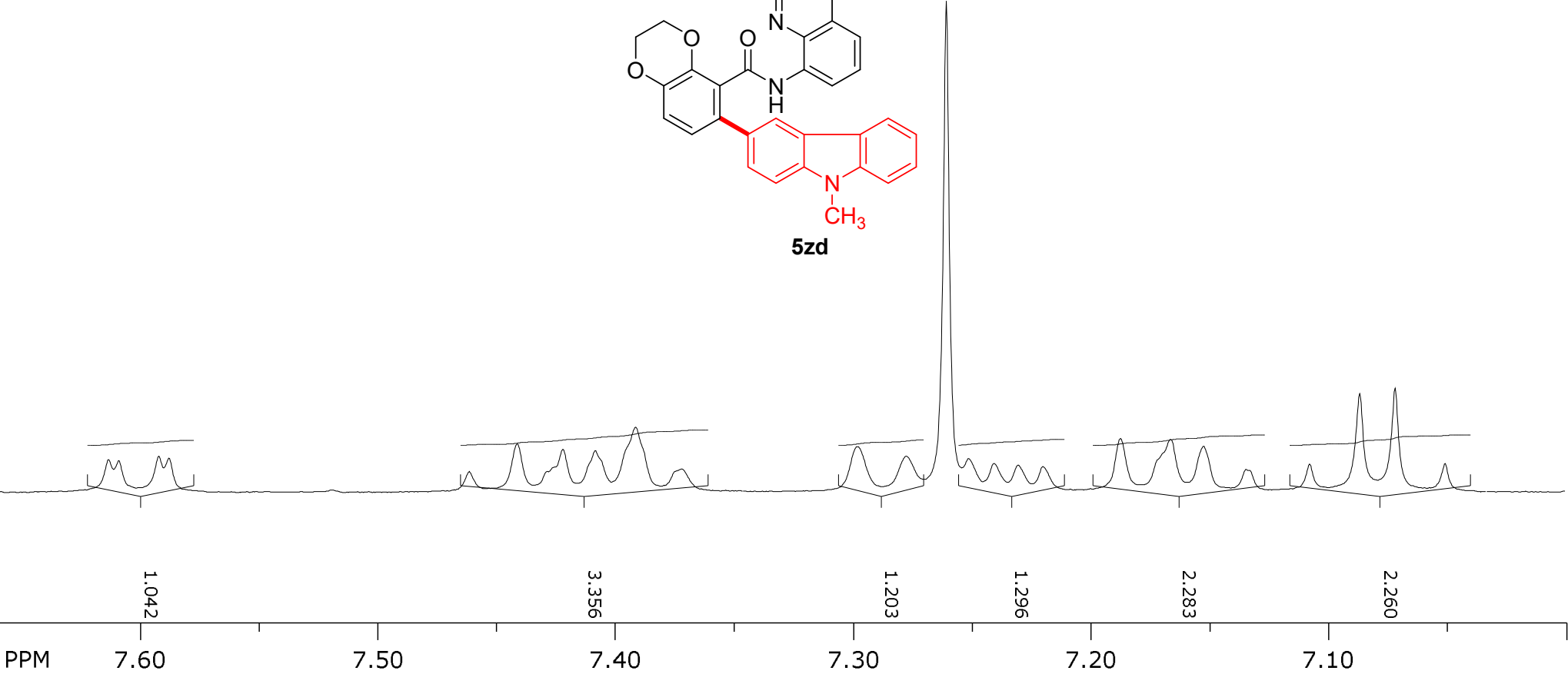
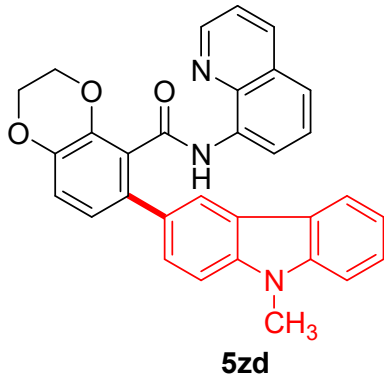


SpinWorks 4: RD-777
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 55



SpinWorks 4: RD-777
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 55

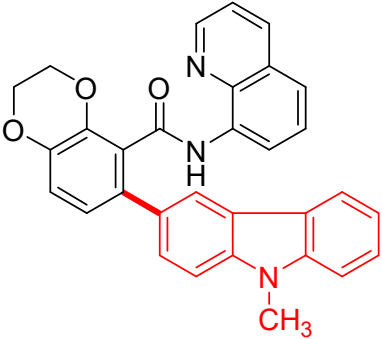
7.0509 —
7.0720 —
7.0869 —
7.1079 —
7.1332 —
7.1348 —
7.1526 —
7.1665 —
7.1875 —
7.2201 —
7.2306 —
7.2408 —
7.2514 —
7.2609 —
7.2778 —
7.2983 —
7.3722 —
7.3915 —
7.4086 —
7.4222 —
7.4288 —
7.4414 —
7.4616 —
7.5880 —
7.5923 —
7.6091 —
7.6134 —



SpinWorks 4: RD-777
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 55

4.3731

3.6791



5zd

4.497

3.345

205

PPM

4.8

4.4

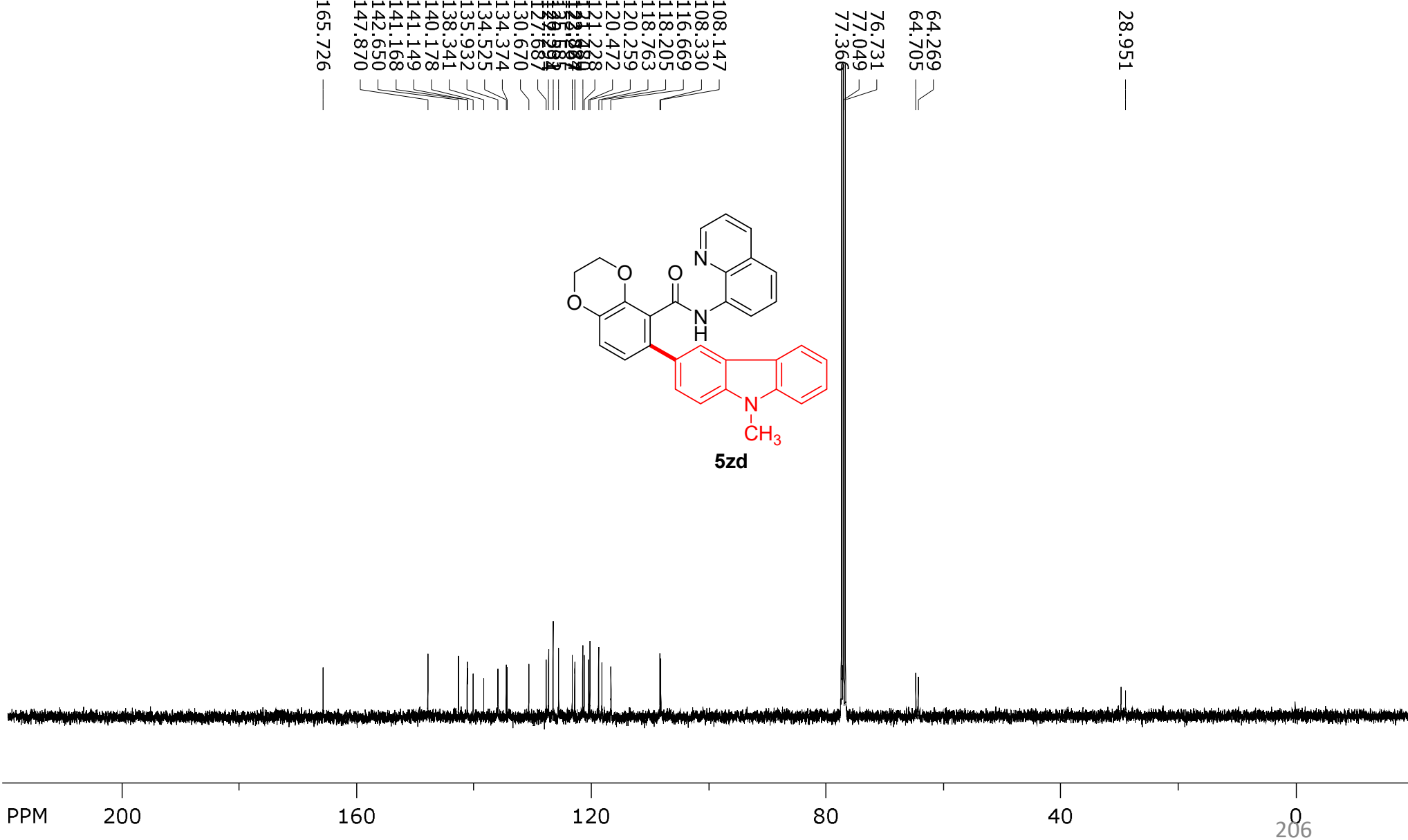
4.0

3.6

3.2

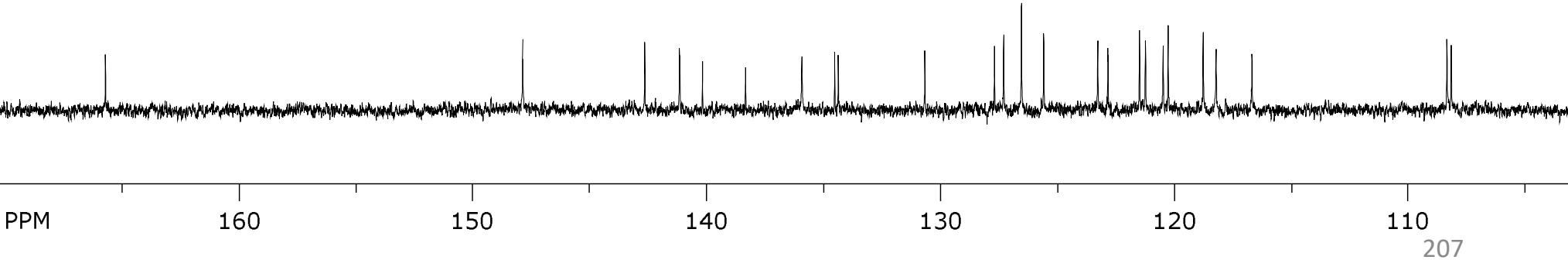
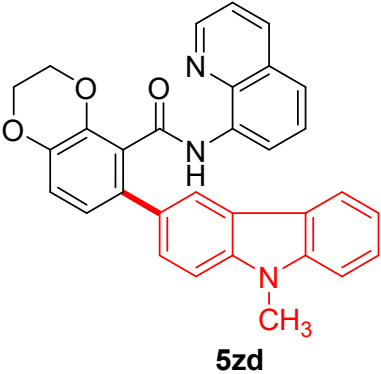
SpinWorks 4: RD-777

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40



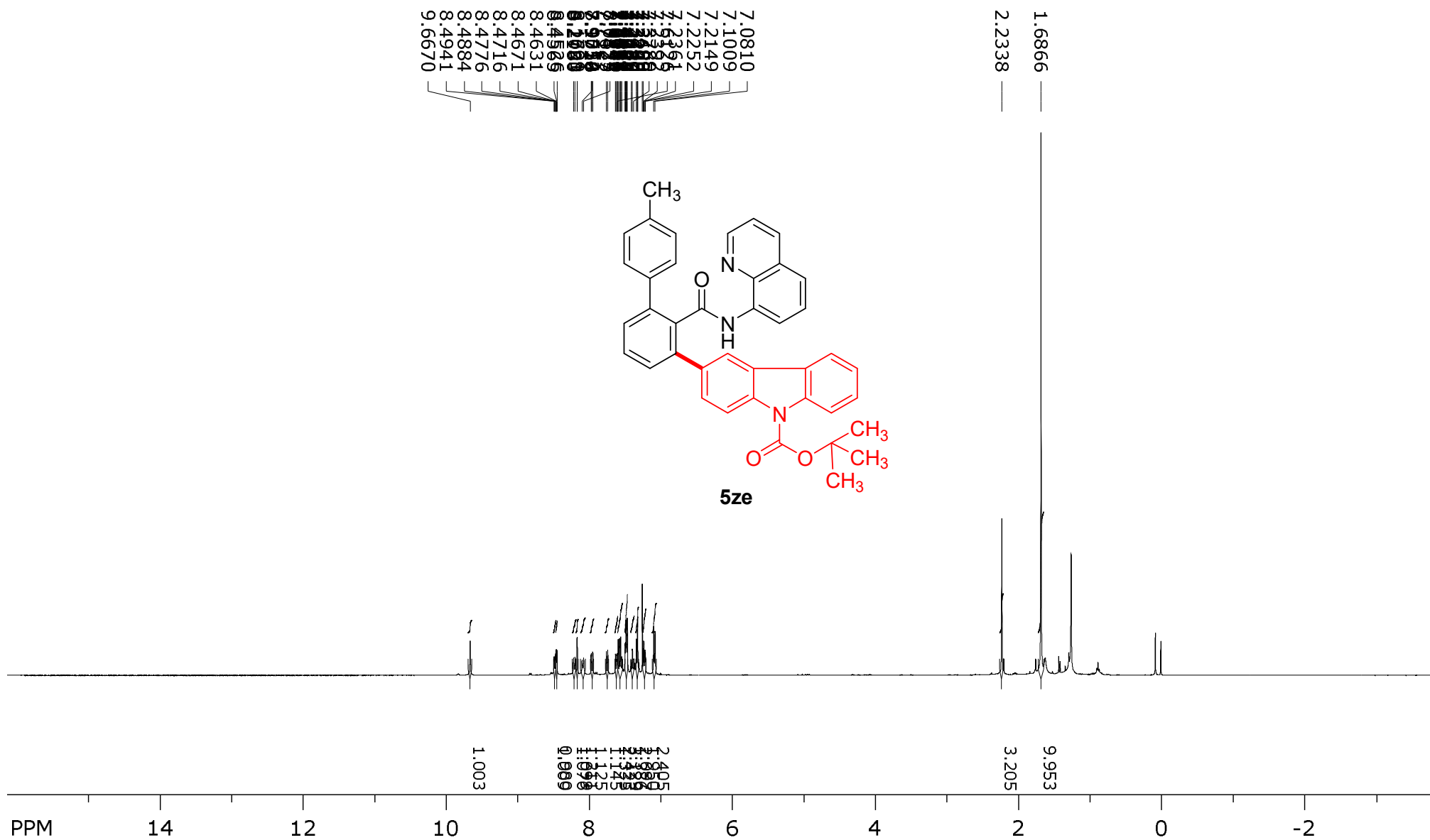
SpinWorks 4: RD-777
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

165.726 —
147.870 —
142.650 —
141.168 —
141.149 —
140.178 —
138.341 —
135.932 —
134.525 —
134.374 —
130.670 —
127.687 —
127.294 —
126.531 —
125.585 —
123.267 —
122.837 —
122.824 —
121.480 —
121.228 —
120.472 —
120.259 —
118.763 —
118.205 —
116.669 —
108.147 —
108.330 —



SpinWorks 4: RD-453A

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9



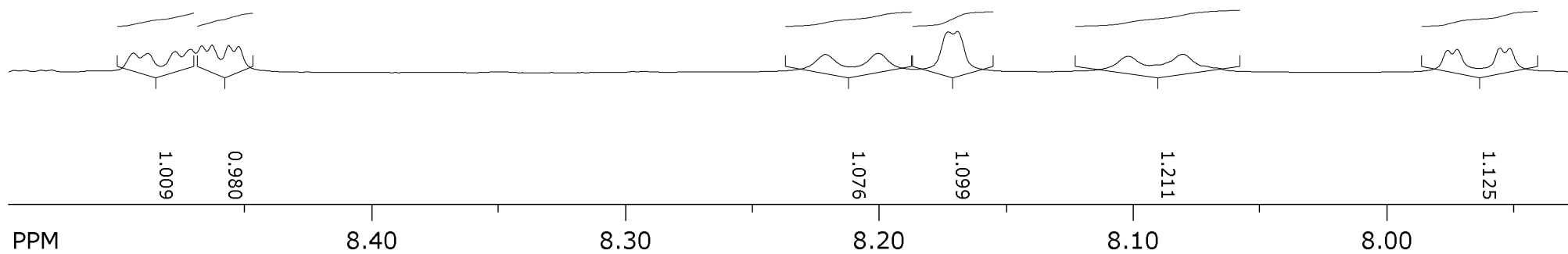
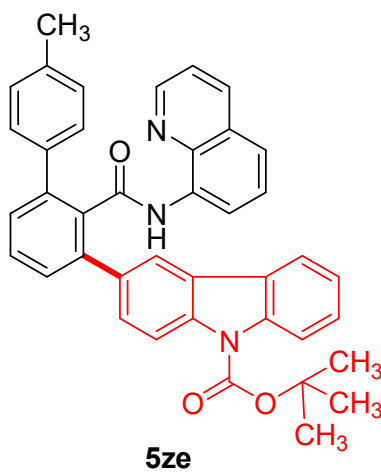
SpinWorks 4: RD-453A
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

8.4526
8.4565
8.4631
8.4671
8.4716
8.4776
8.4884
8.4941

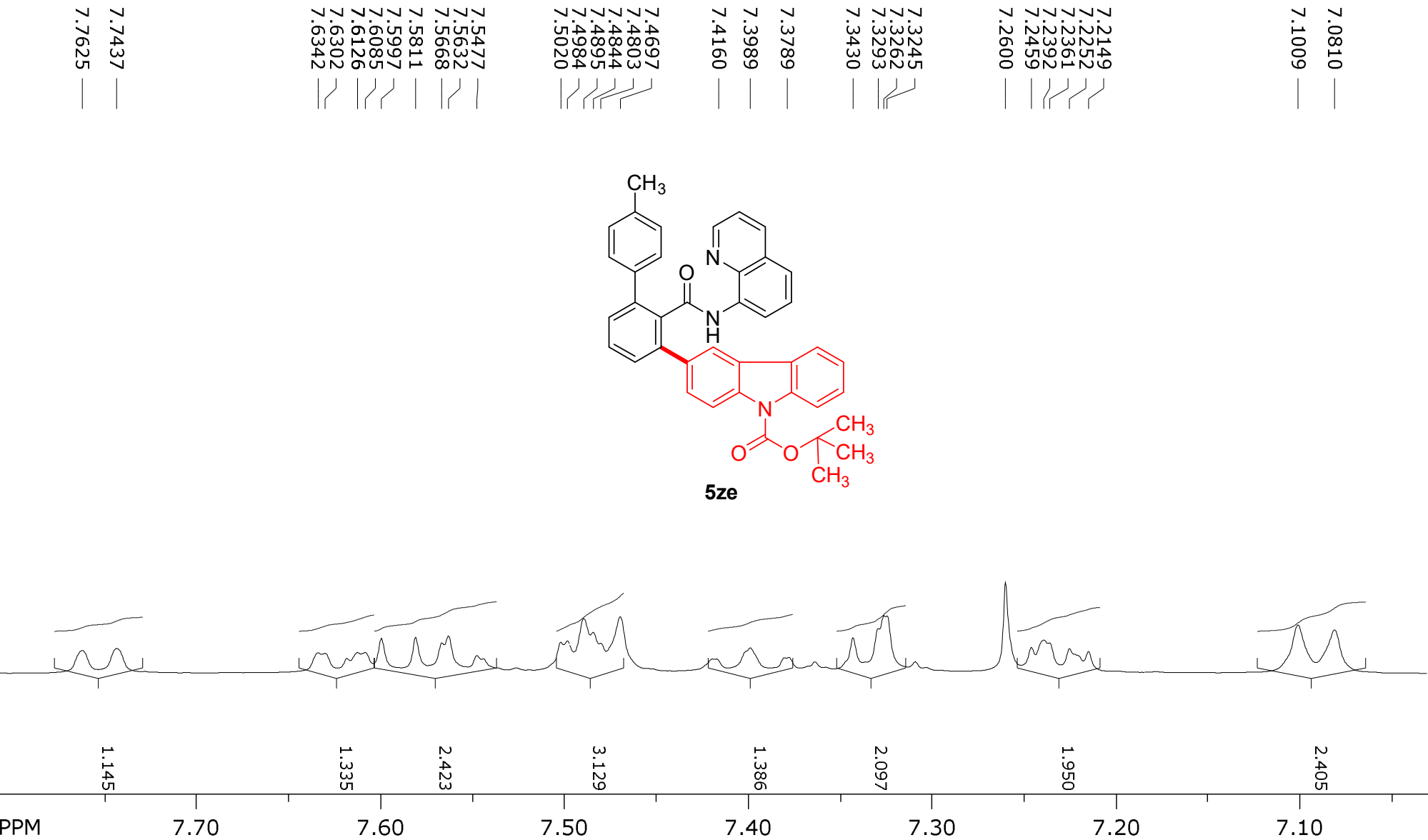
8.2180
8.2003
8.1729
8.1691

8.1016
8.0825

7.9720
7.9758
7.9552
7.9514

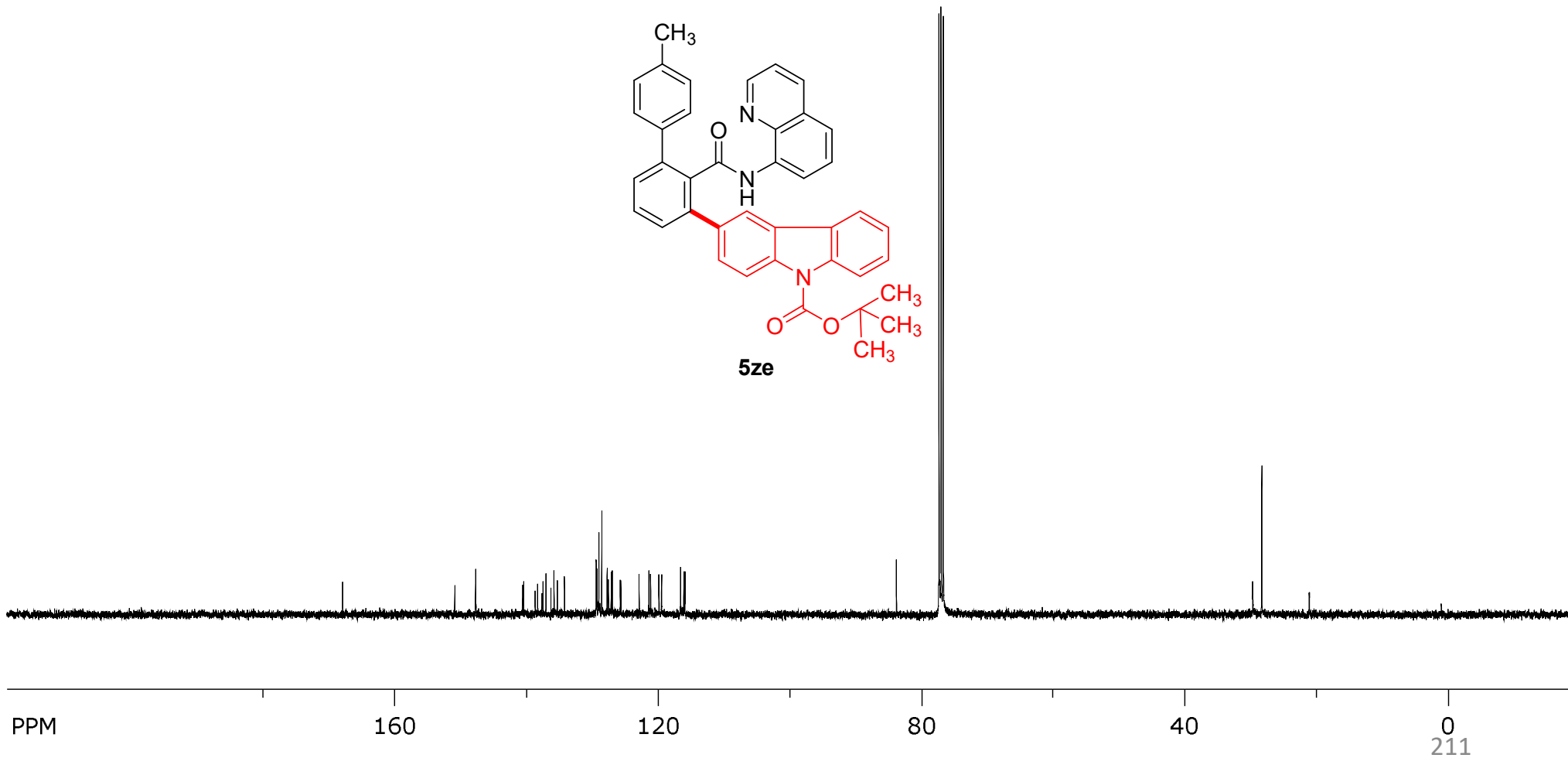
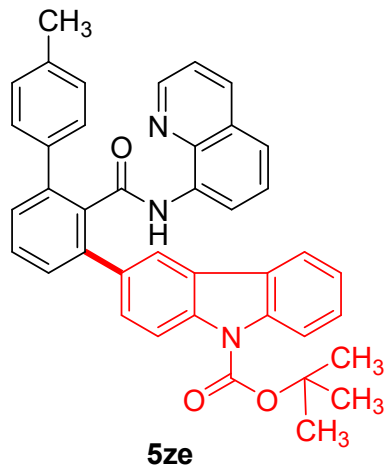


SpinWorks 4: RD-453A
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9



SpinWorks 4: RD-453A
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

167.913	150.895	147.737	140.599	140.416	138.679	138.301	137.660	137.479	134.325	134.049	133.825	129.825	129.825	129.825	129.825	122.882	121.394	121.150	119.883	119.478	116.582	116.092	115.926	83.797	77.338	77.020	76.703	28.307	21.098
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SpinWorks 4: RD-453A

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

167.913

150.895

147.737

140.599

140.416

138.301

137.660

137.479

137.047

136.294

135.810

134.225

129.416

129.402

129.294

128.998

128.568

127.752

127.538

127.140

126.972

125.739

125.650

122.882

121.394

121.150

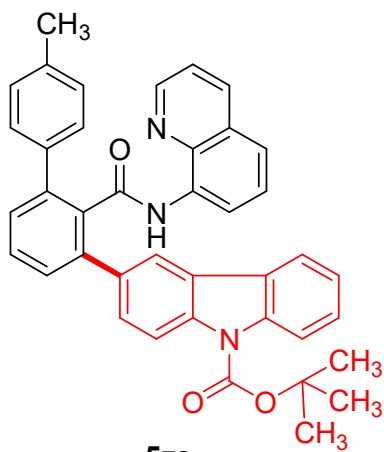
119.883

119.478

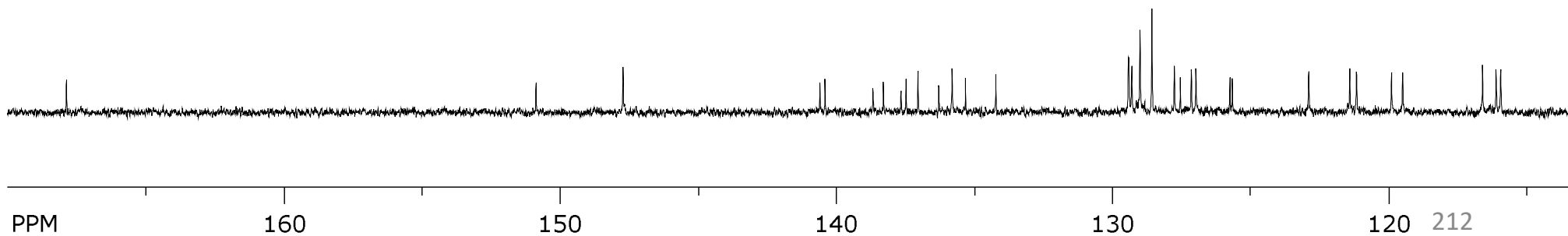
116.582

116.092

115.926



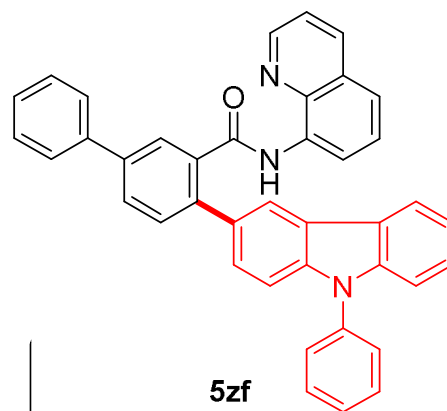
5ze



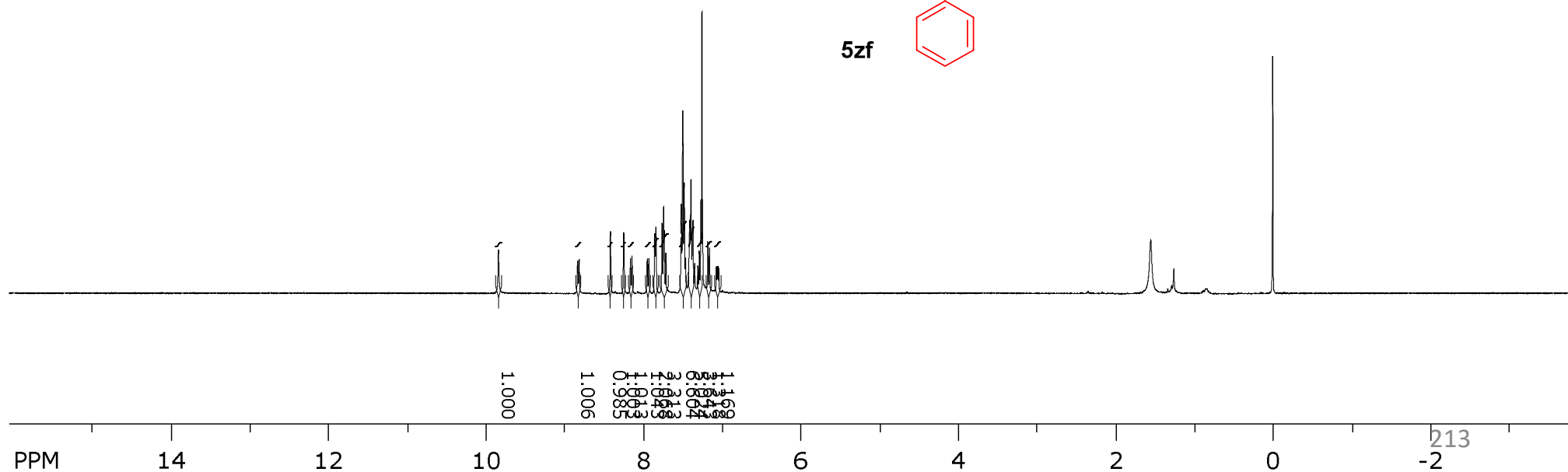
SpinWorks 4: RD-1115

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

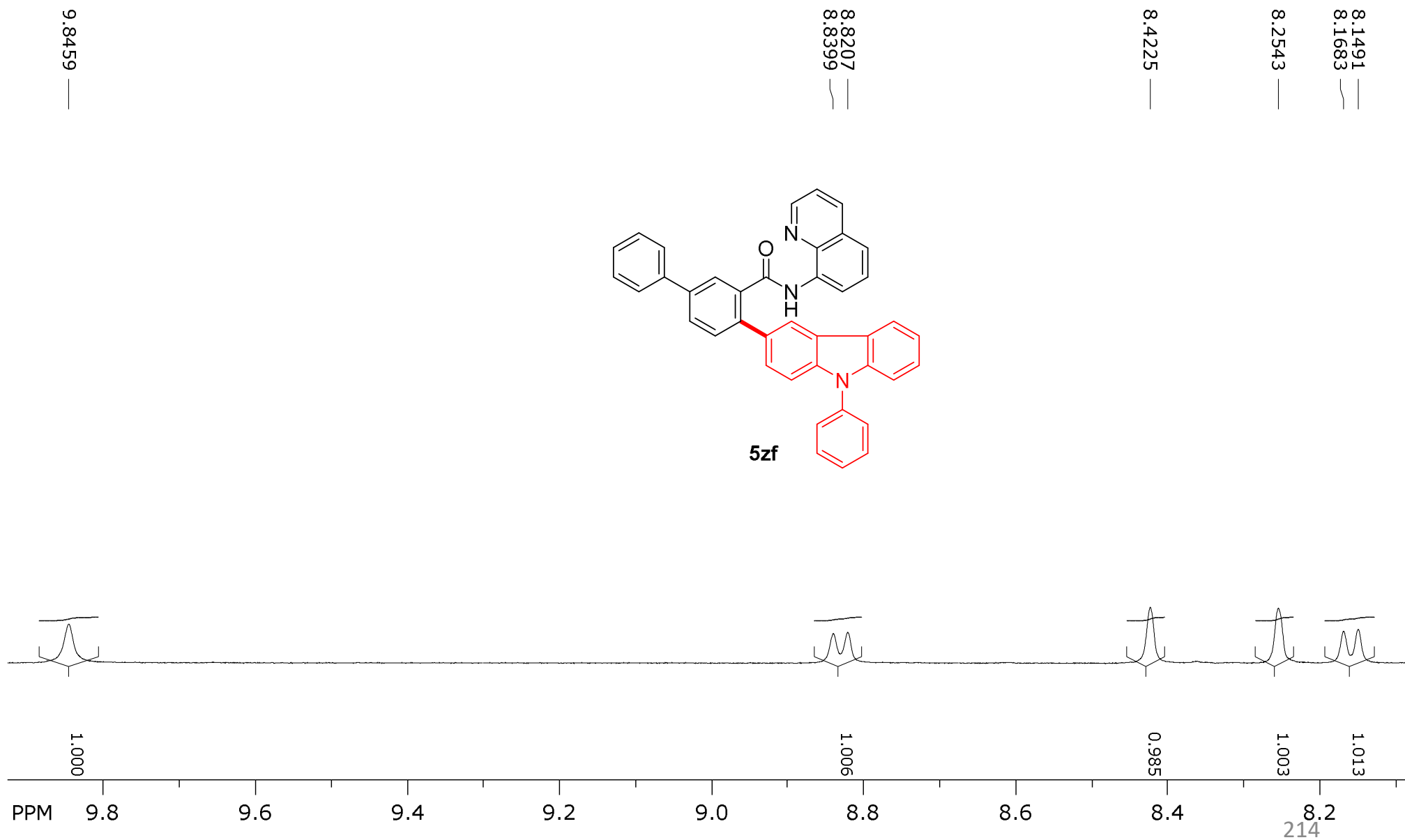
7.0466
7.0572
7.0672
7.0776
7.1634
7.1845
7.2600
7.9343
7.9549
8.1491
8.1683
8.2543
8.4225
8.8207
8.8399
9.8459



5zf



SpinWorks 4: RD-1115
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: RD-1115

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

7.9343 —
7.9549 —

7.8454 —
7.8591 —

7.7185 —
7.7391 —
7.7469 —
7.7664 —

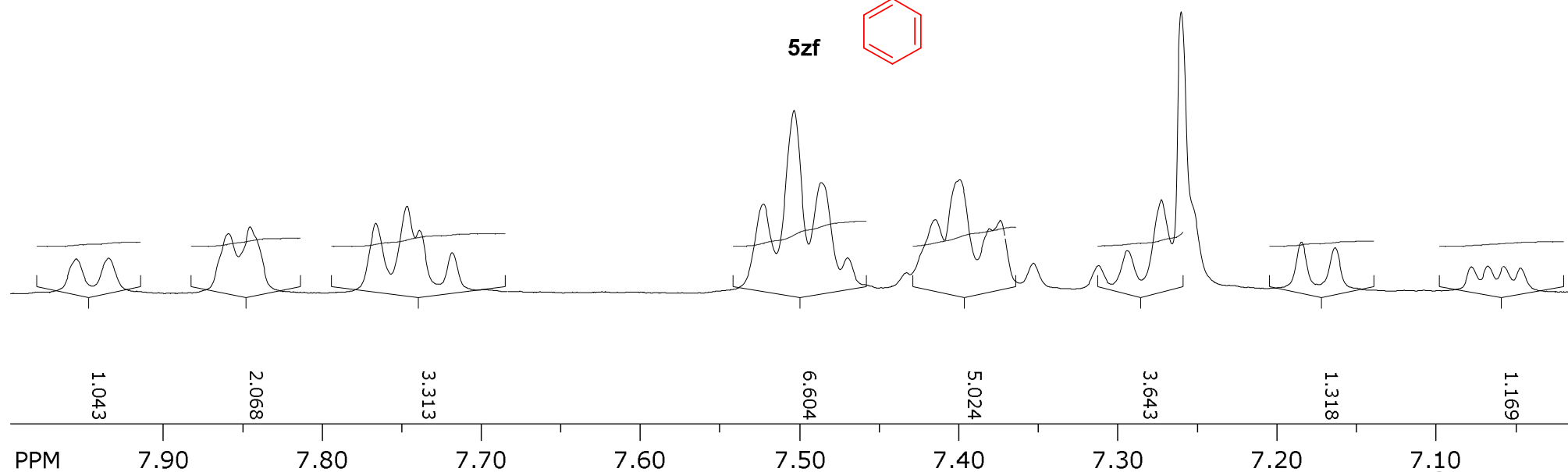
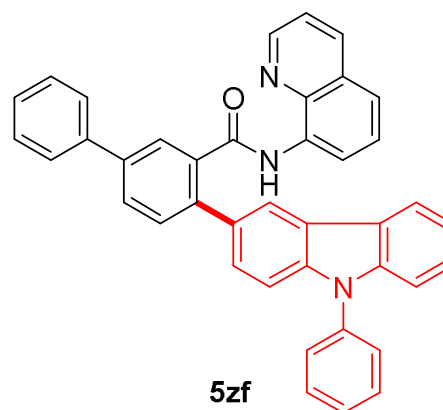
7.4699 —
7.4865 —
7.5035 —
7.5228 —

7.3736 —
7.3807 —
7.3993 —
7.4147 —

7.2600 —
7.2725 —
7.2939 —
7.3120 —

7.1634 —
7.1845 —

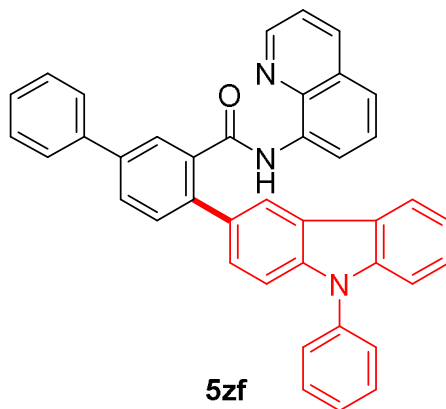
7.0466 —
7.0572 —
7.0672 —
7.0776 —



SpinWorks 4: RD-1115

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7

168.024
147.332
141.028
140.486
140.055
139.988
139.836
138.168
137.347
136.980
134.527
131.589
131.587
123.401
123.359
121.412
121.043
120.992
120.365
120.107
116.489
109.771
77.337
77.020
76.702



PPM

160

120

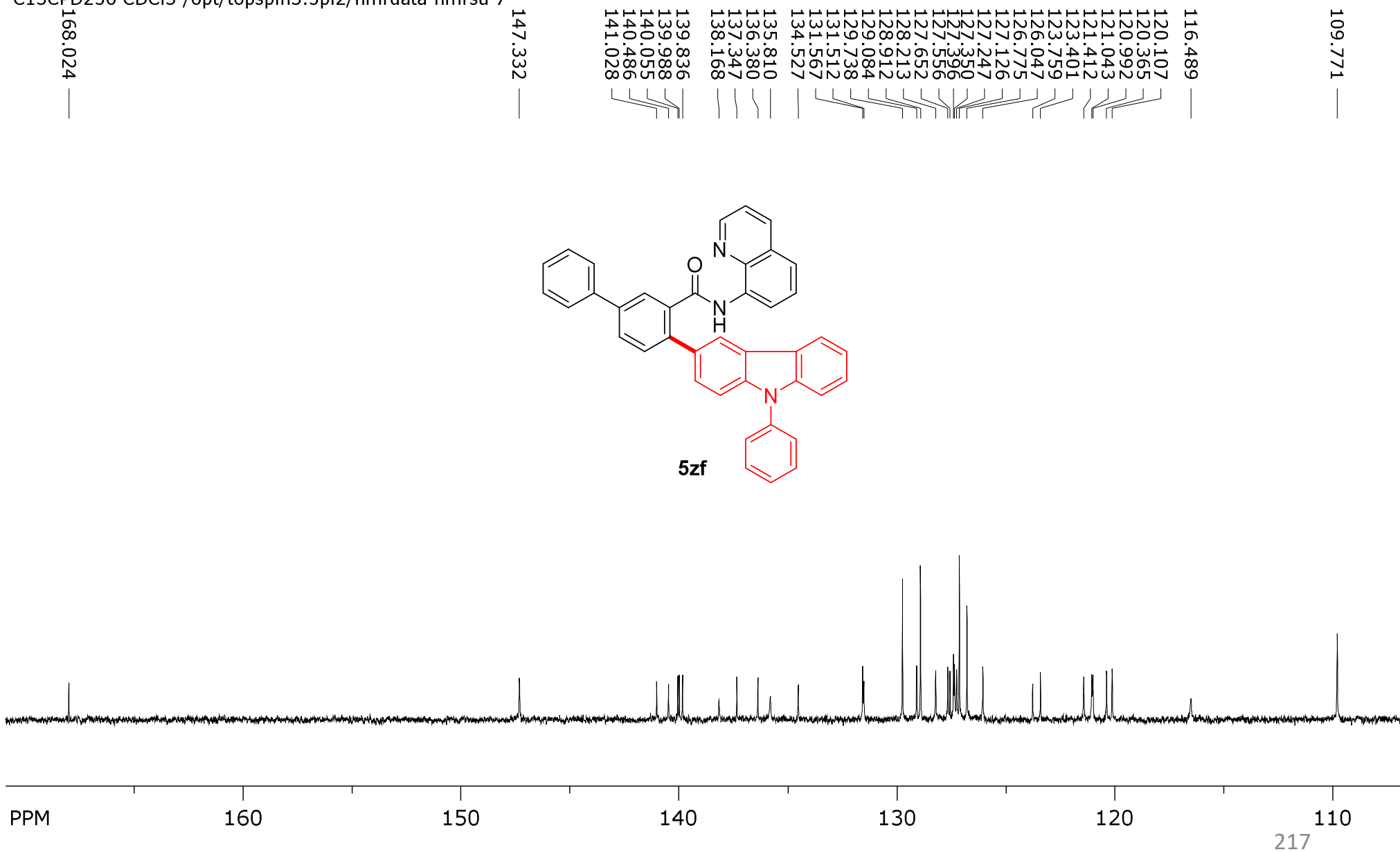
80

40

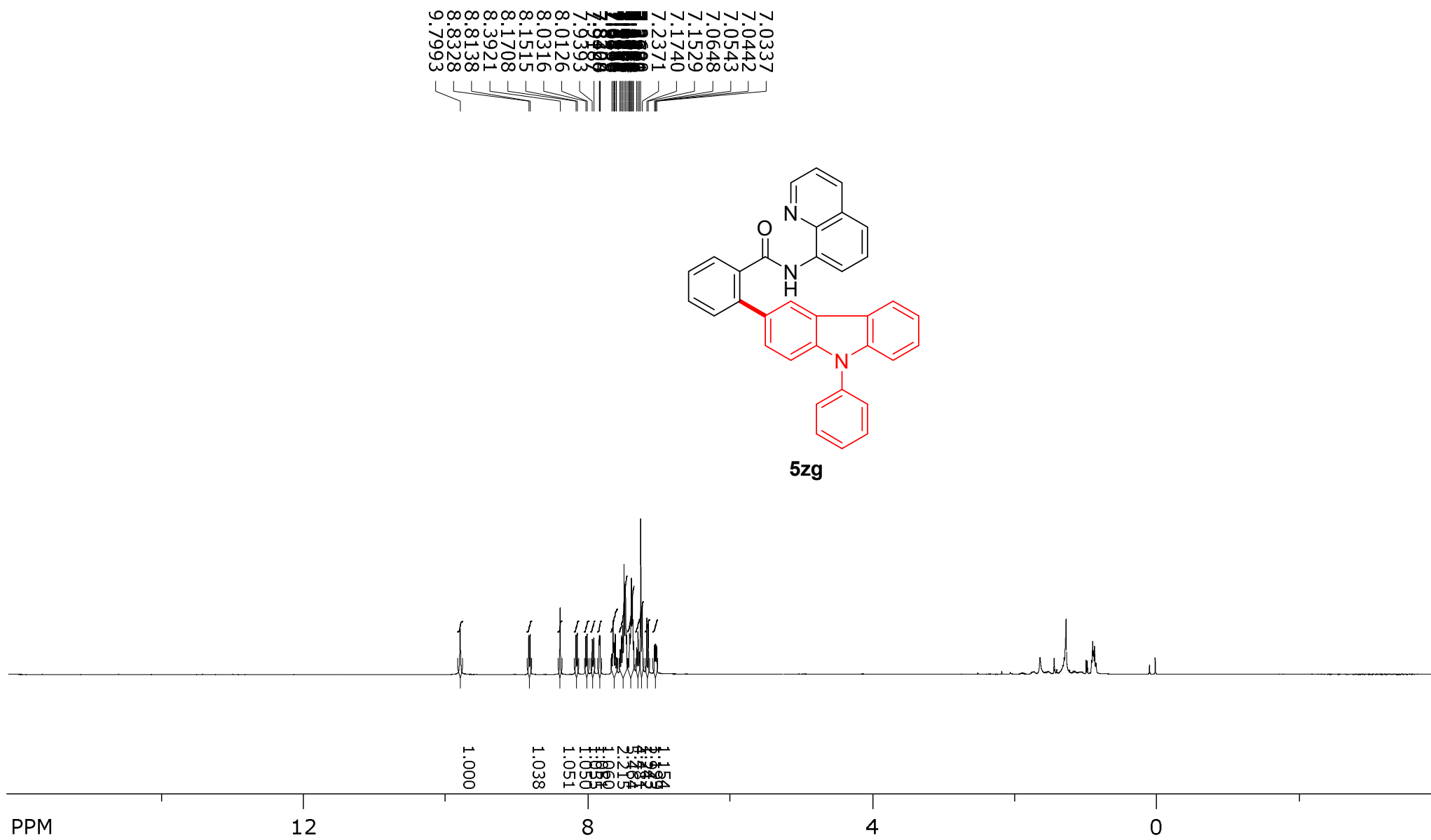
216
0

SpinWorks 4: RD-1115

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 7



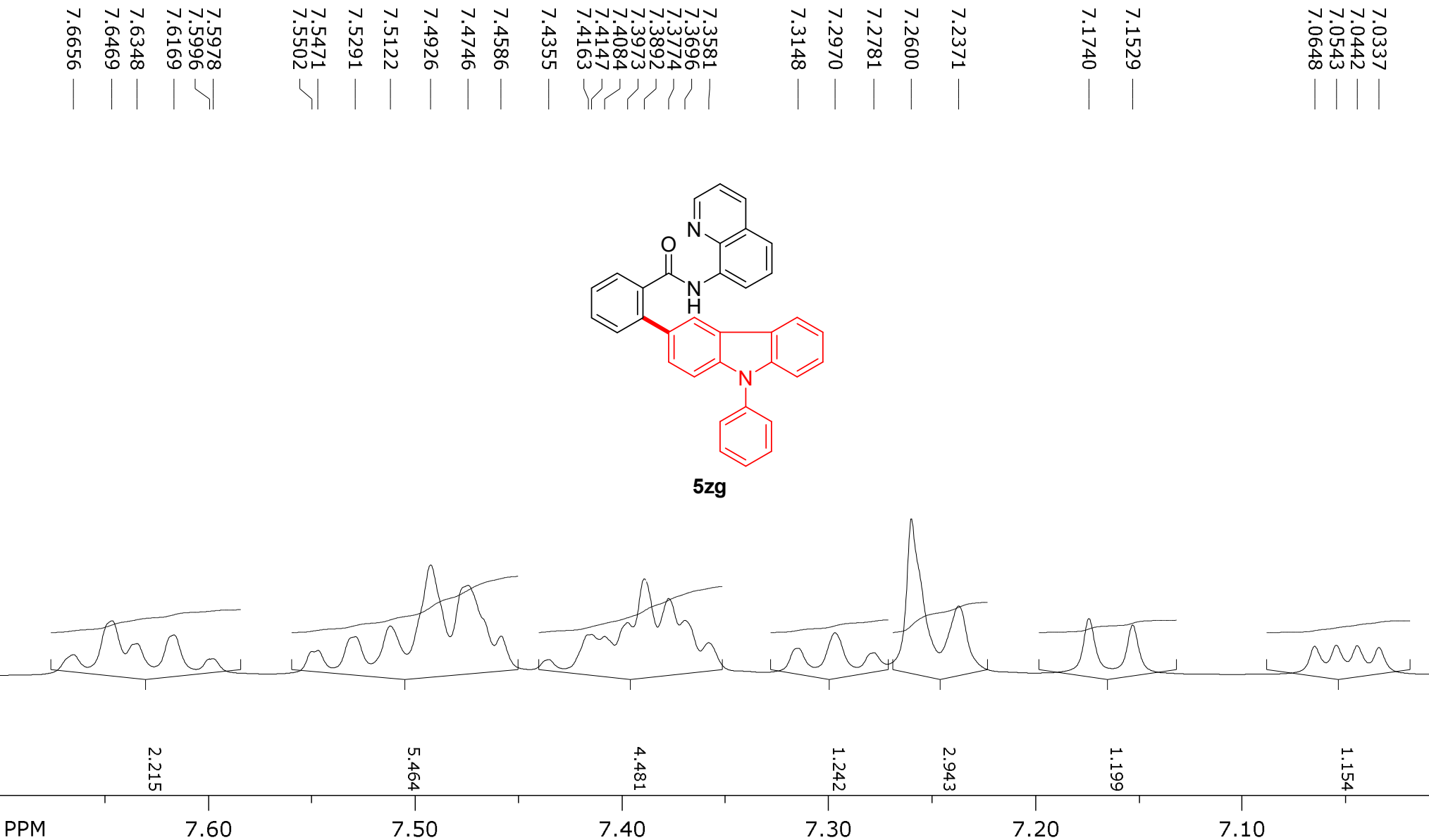
SpinWorks 4: rd-143



SpinWorks 4: rd-143



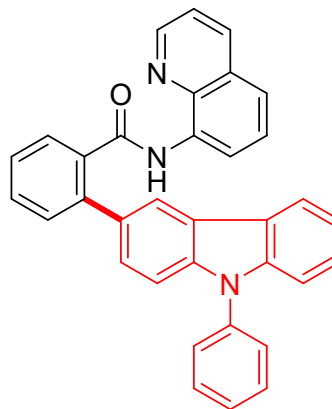
SpinWorks 4: rd-143



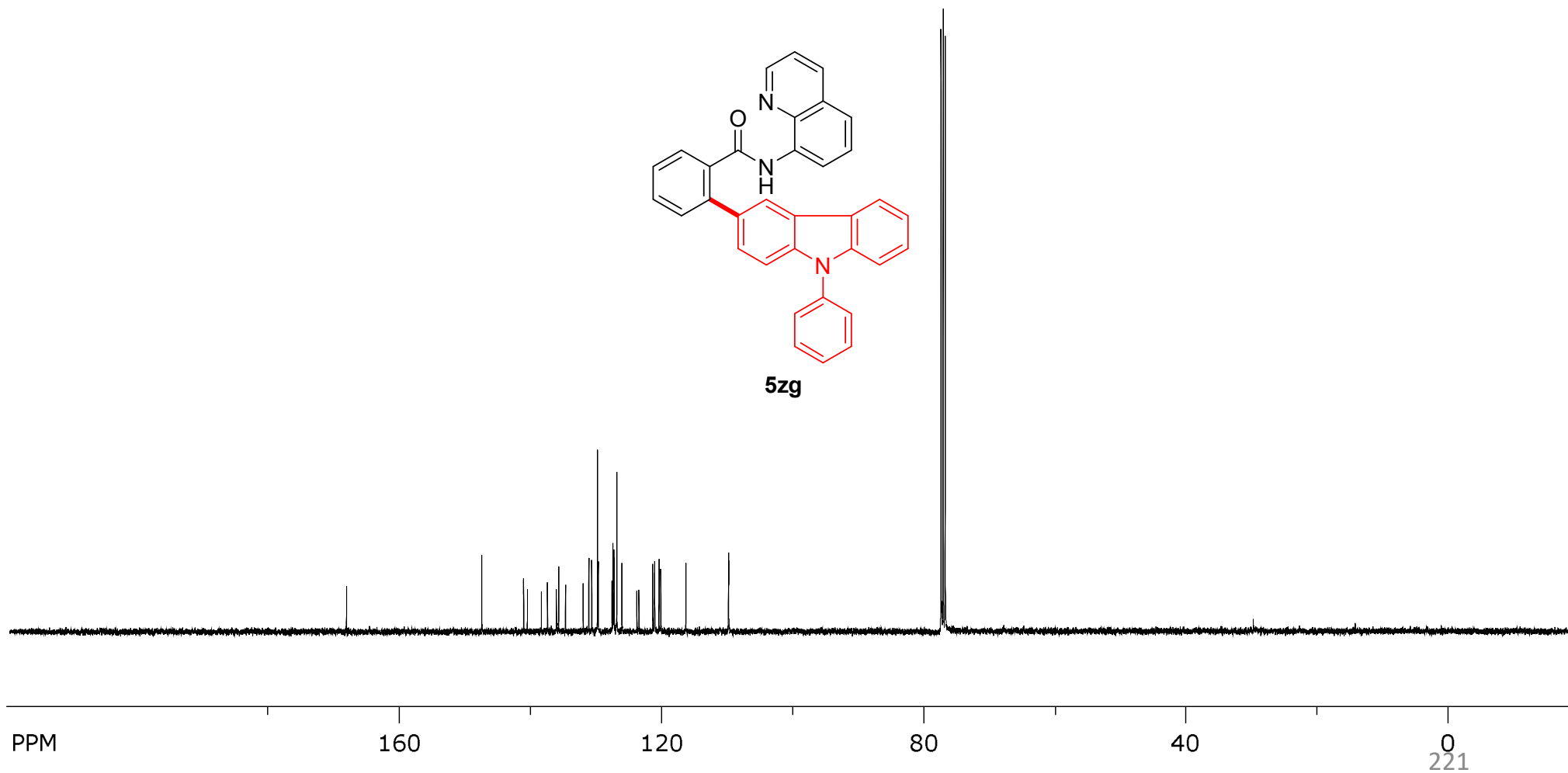
SpinWorks 4: RD 143

C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata/nmr su 3

109.727
109.756
116.254
120.077
120.359
121.001
121.048
121.313
123.745
123.809
123.889
123.909
133.618
134.618
135.651
135.997
137.361
138.288
140.437
140.994
141.014
147.388
76.703
77.020
77.338
68.023

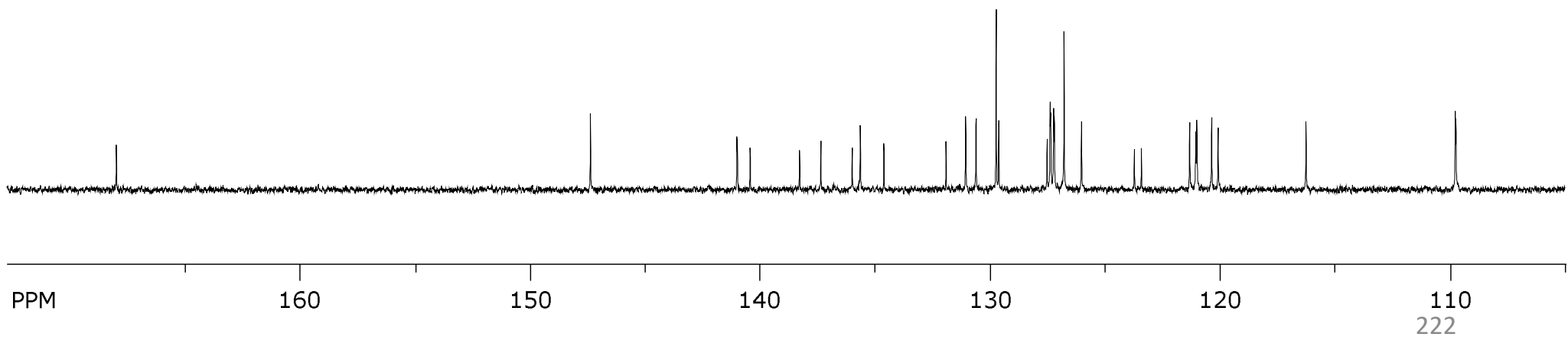
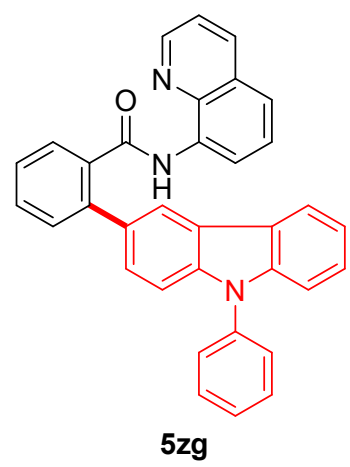


5zg

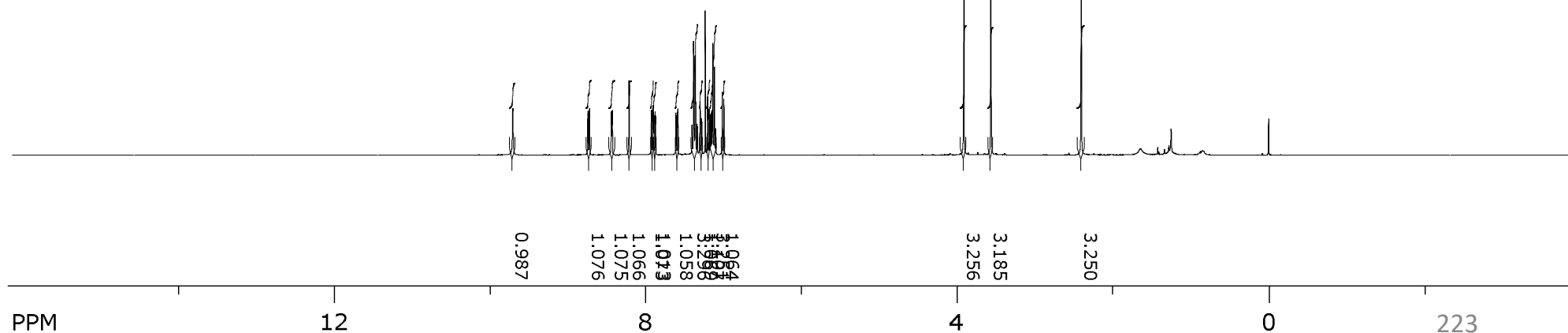
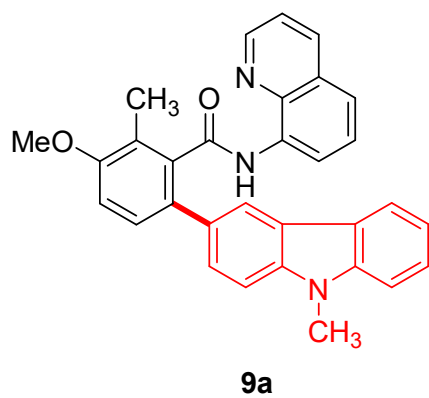
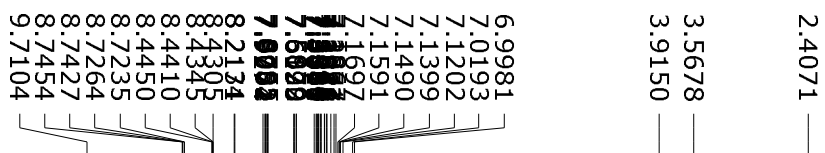


SpinWorks 4: RD 143
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

168.023 —
147.388 —
140.437 —
140.994 —
141.014 —
138.288 —
137.361 —
135.997 —
135.651 —
134.618 —
131.915 —
131.061 —
130.613 —
129.736 —
129.620 —
127.520 —
127.385 —
127.364 —
127.233 —
127.203 —
126.782 —
126.018 —
123.725 —
123.416 —
121.313 —
121.048 —
121.001 —
120.359 —
120.077 —
116.254 —
109.727 —
109.756 —

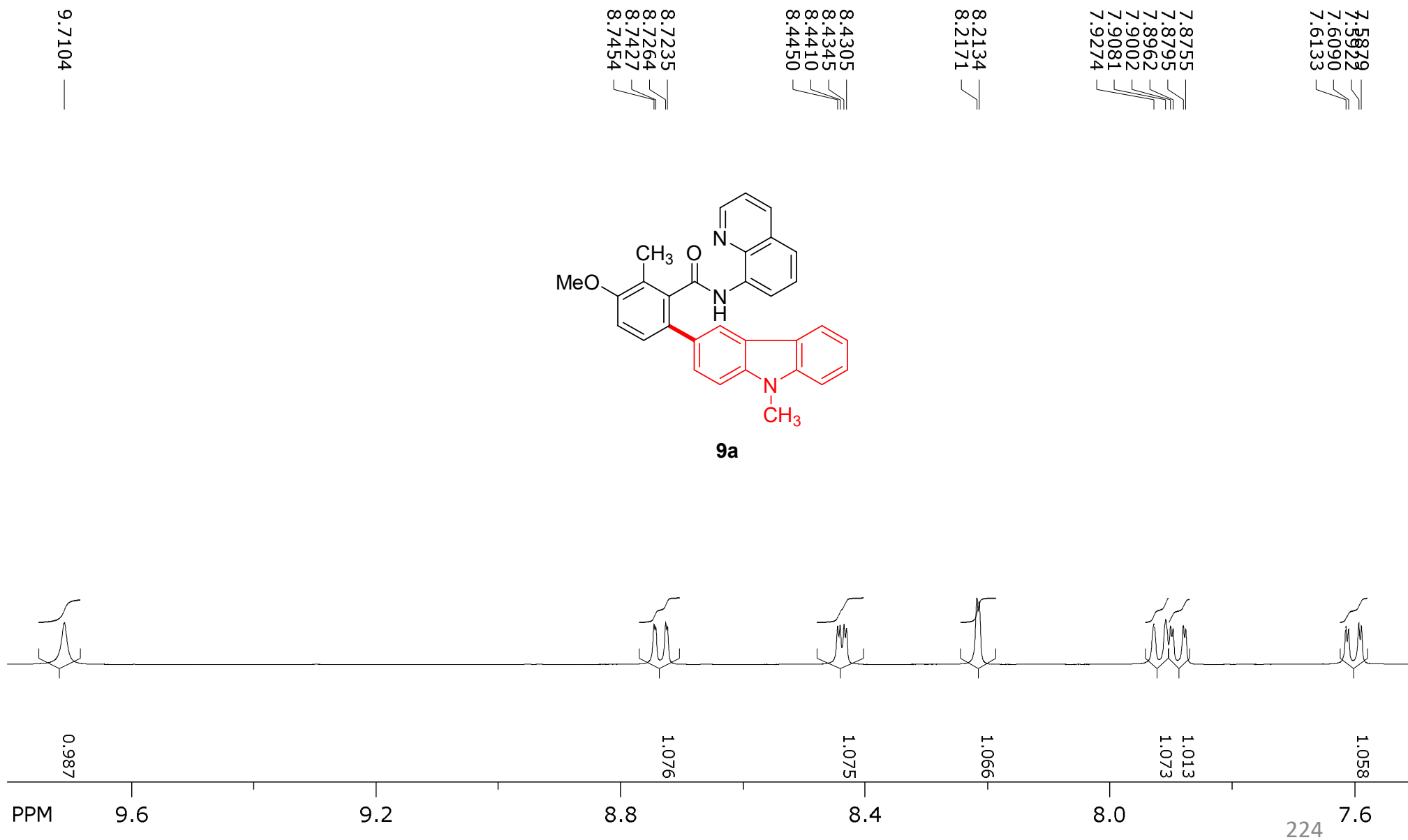


PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



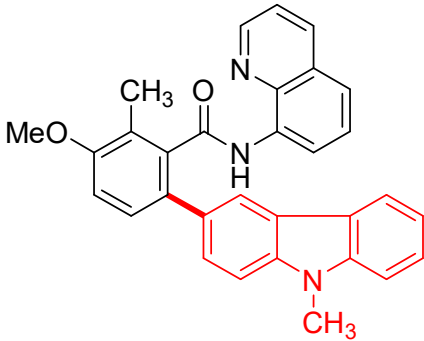
SpinWorks 4: RD-1212

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 1

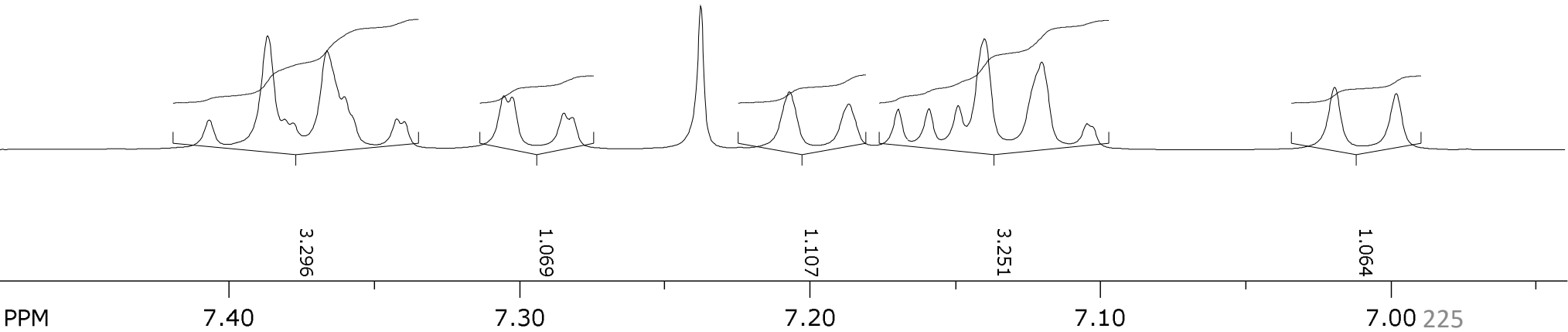


SpinWorks 4: RD-1212
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

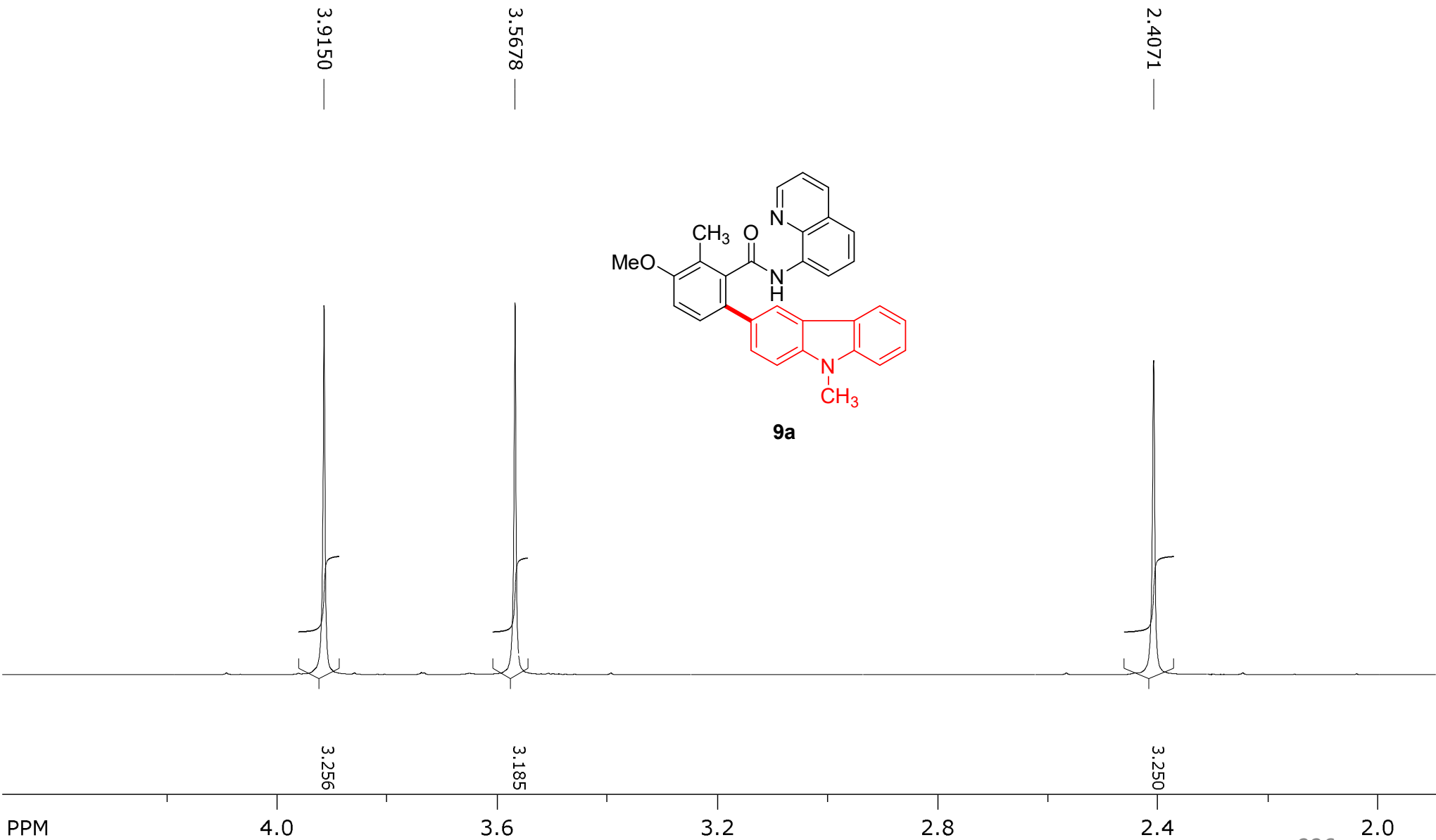
7.4070	7.3869	7.3665	7.3424	7.3398	7.3027	7.3055	7.2820	7.2848	7.2377	7.2071	7.1867	7.1697	7.1591	7.1490	7.1399	7.1202	7.0193	6.9981
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



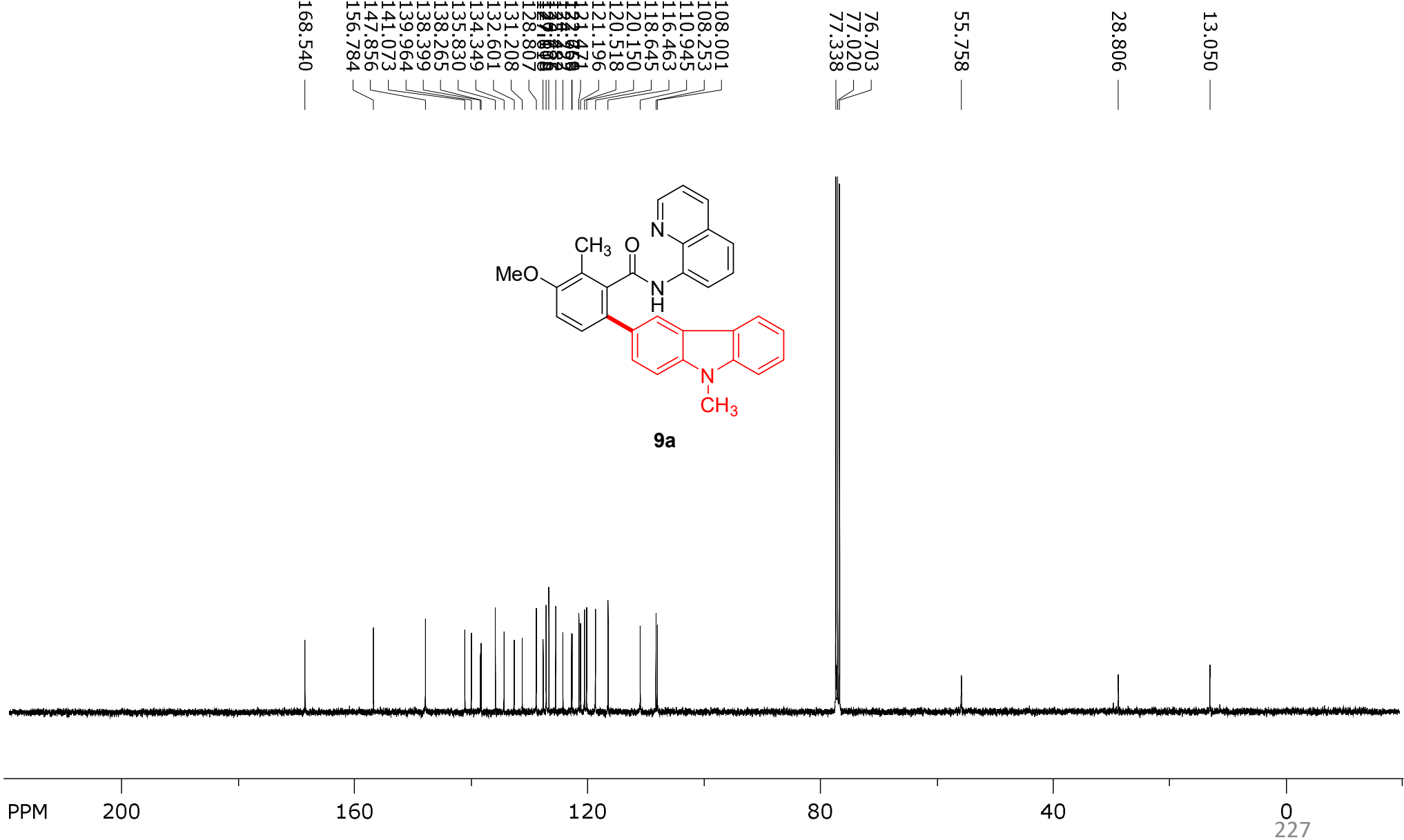
9a



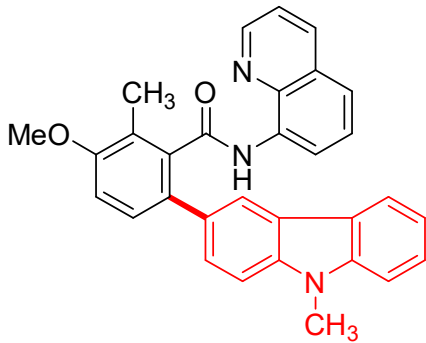
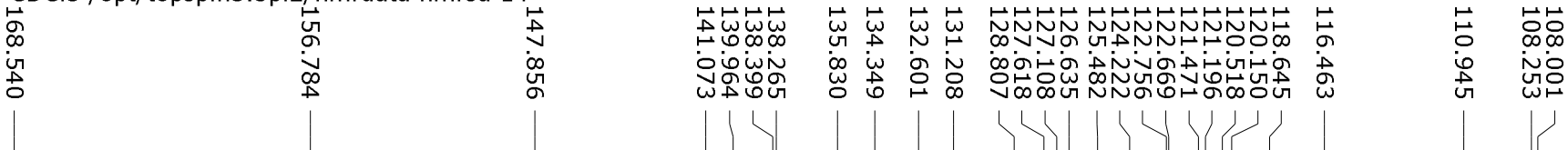
SpinWorks 4: RD-1212
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



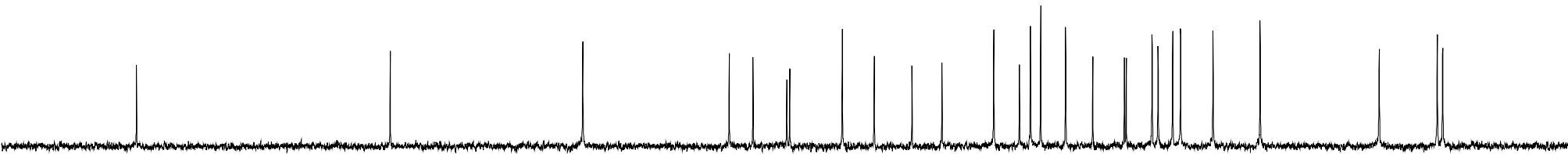
SpinWorks 4: RD-1212
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14



SpinWorks 4: RD-1212
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

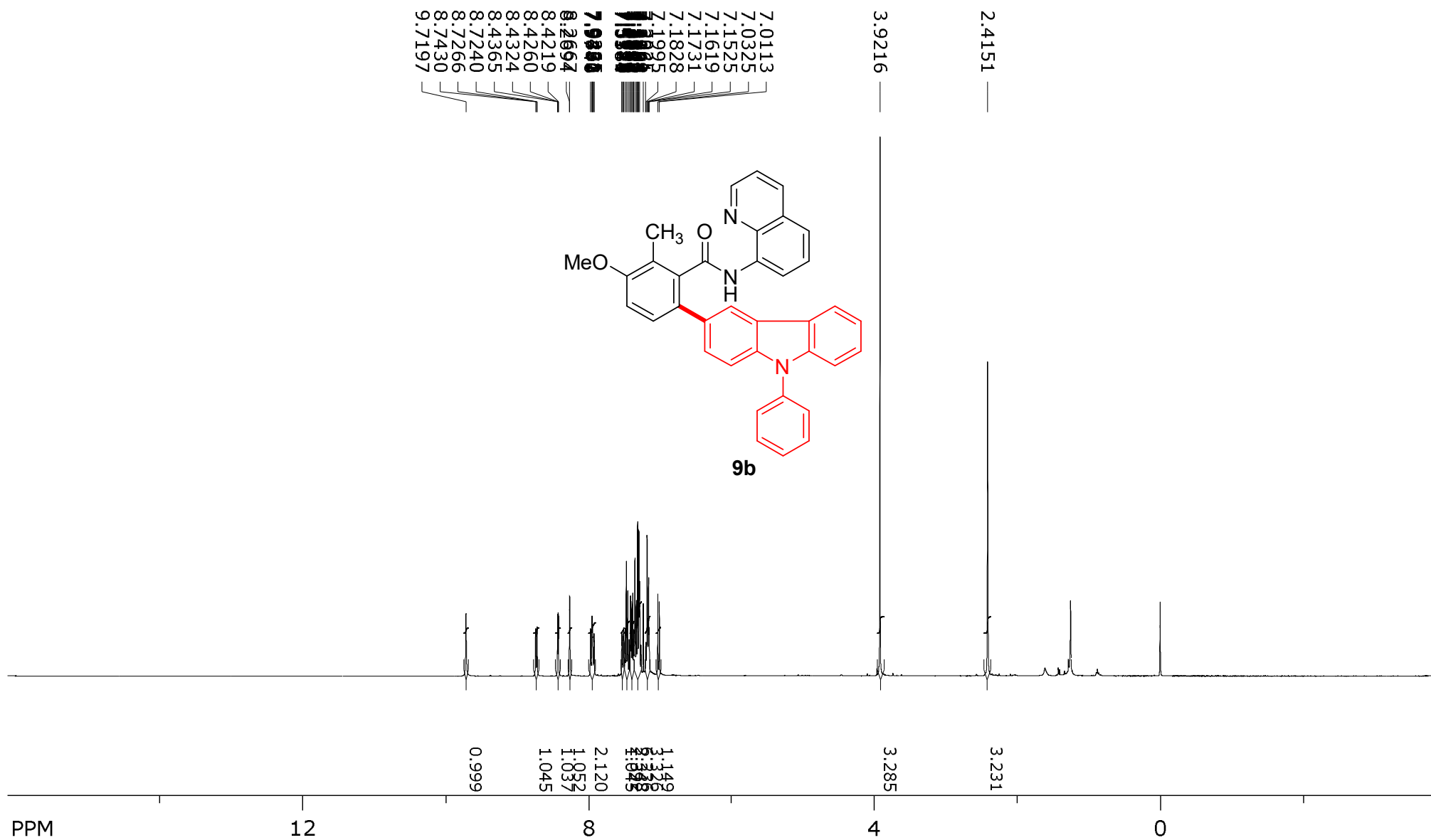


9a

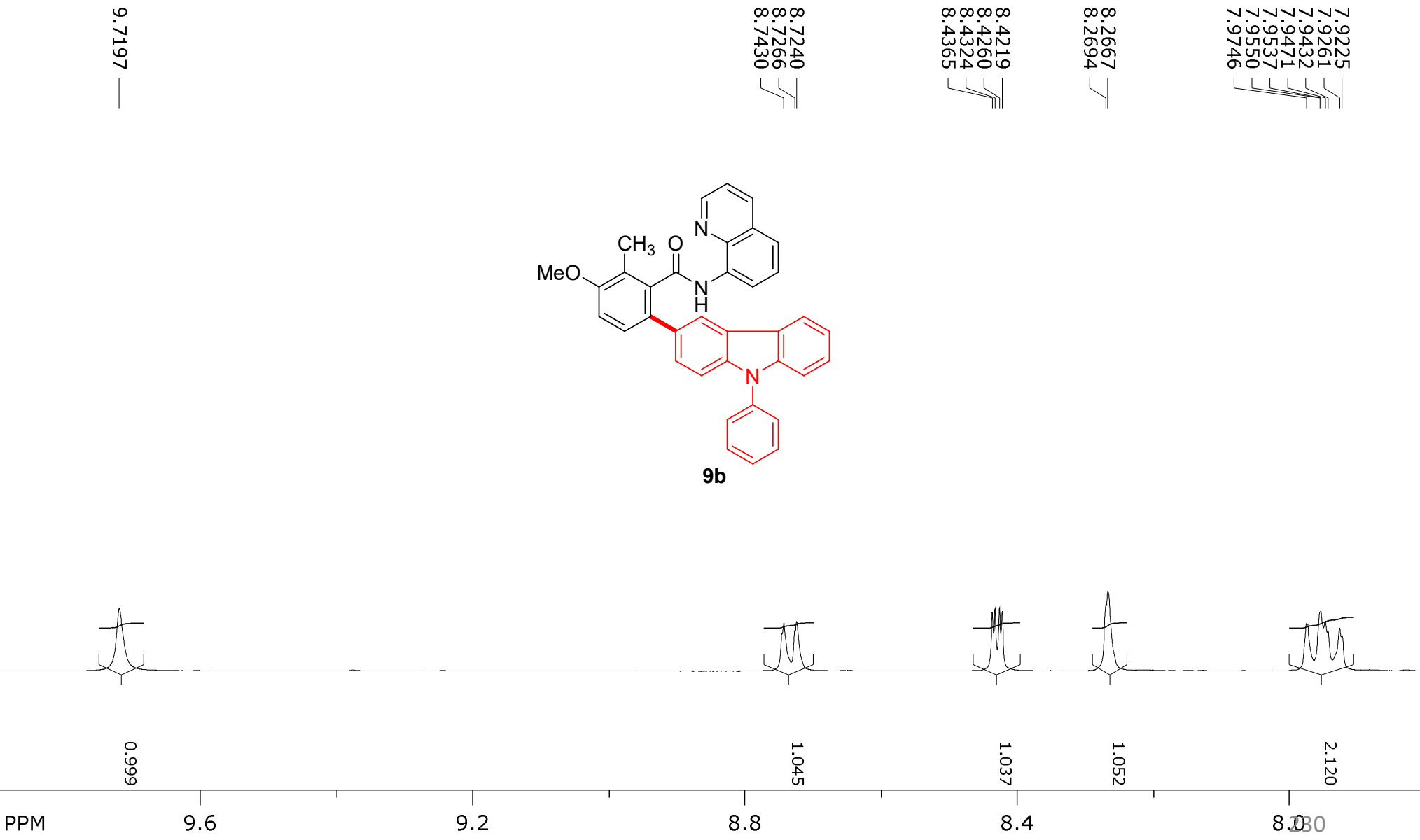


PPM 160 150 140 130 120 110 228

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

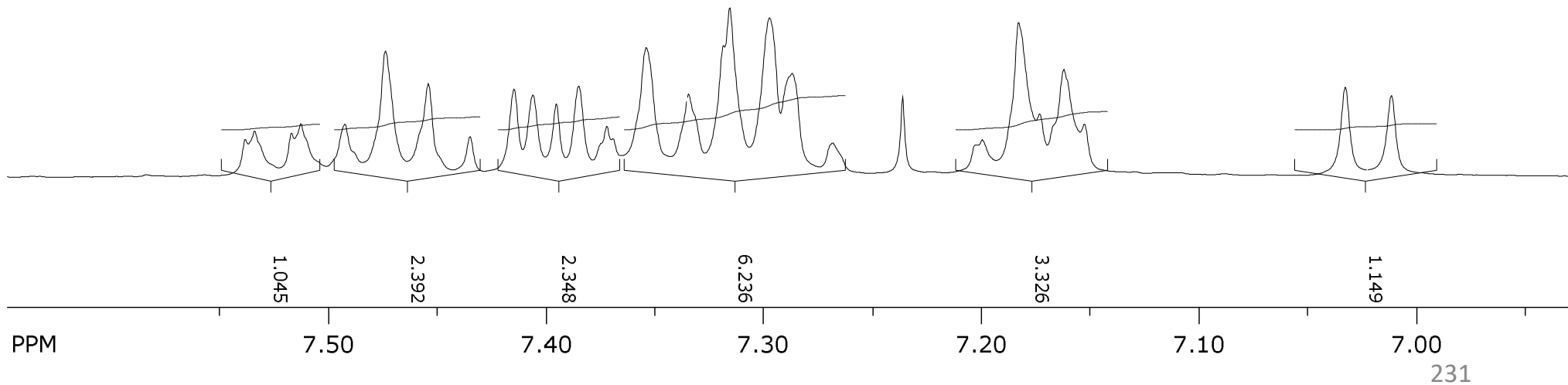
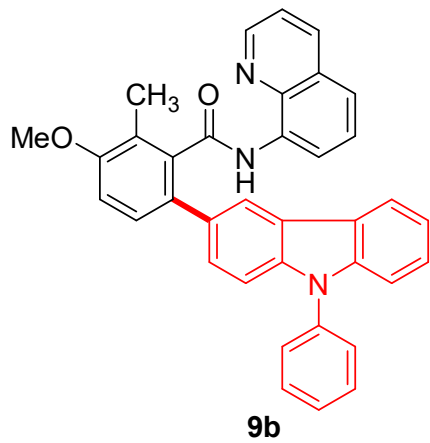


SpinWorks 4: RD-946
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

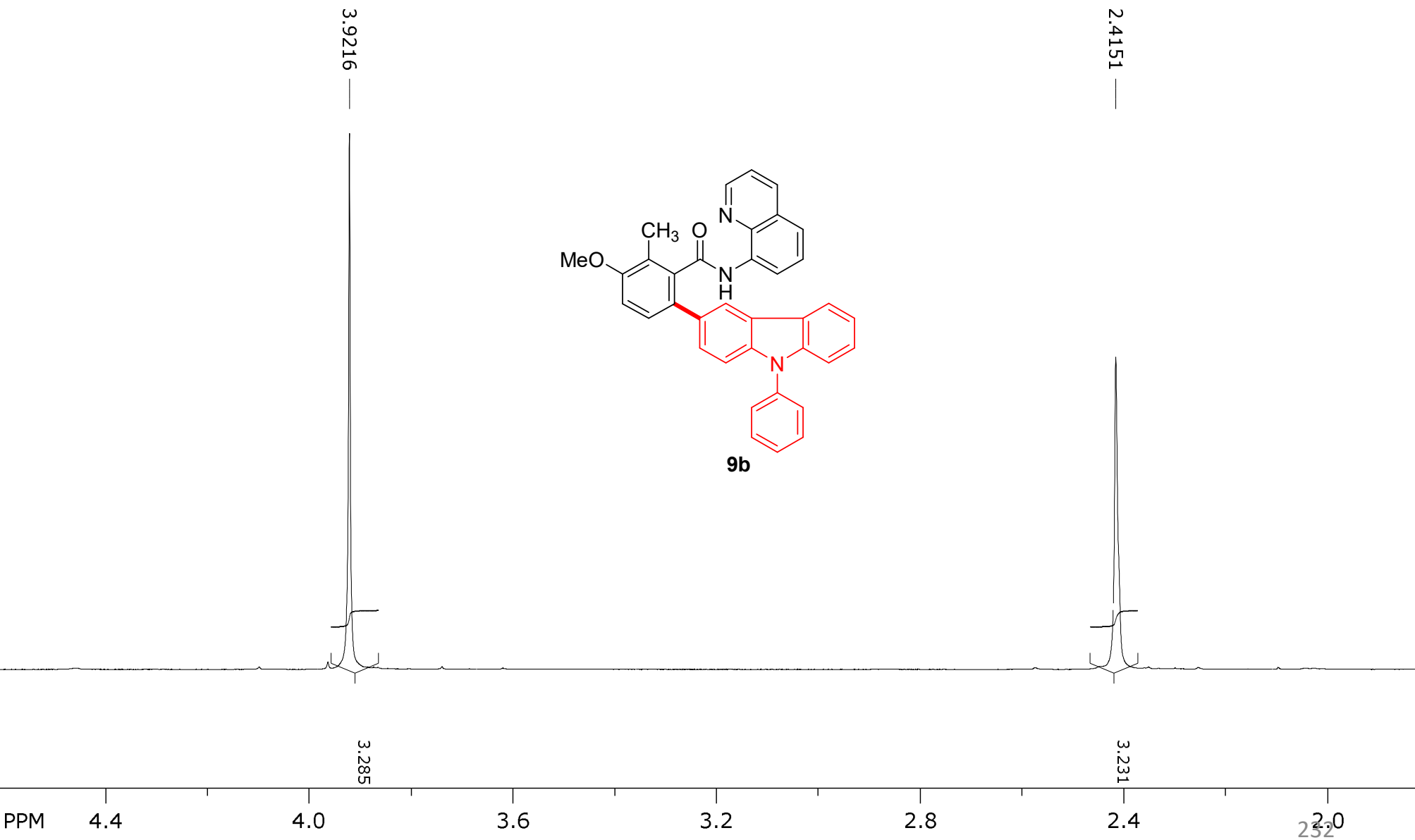


SpinWorks 4: RD-946
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

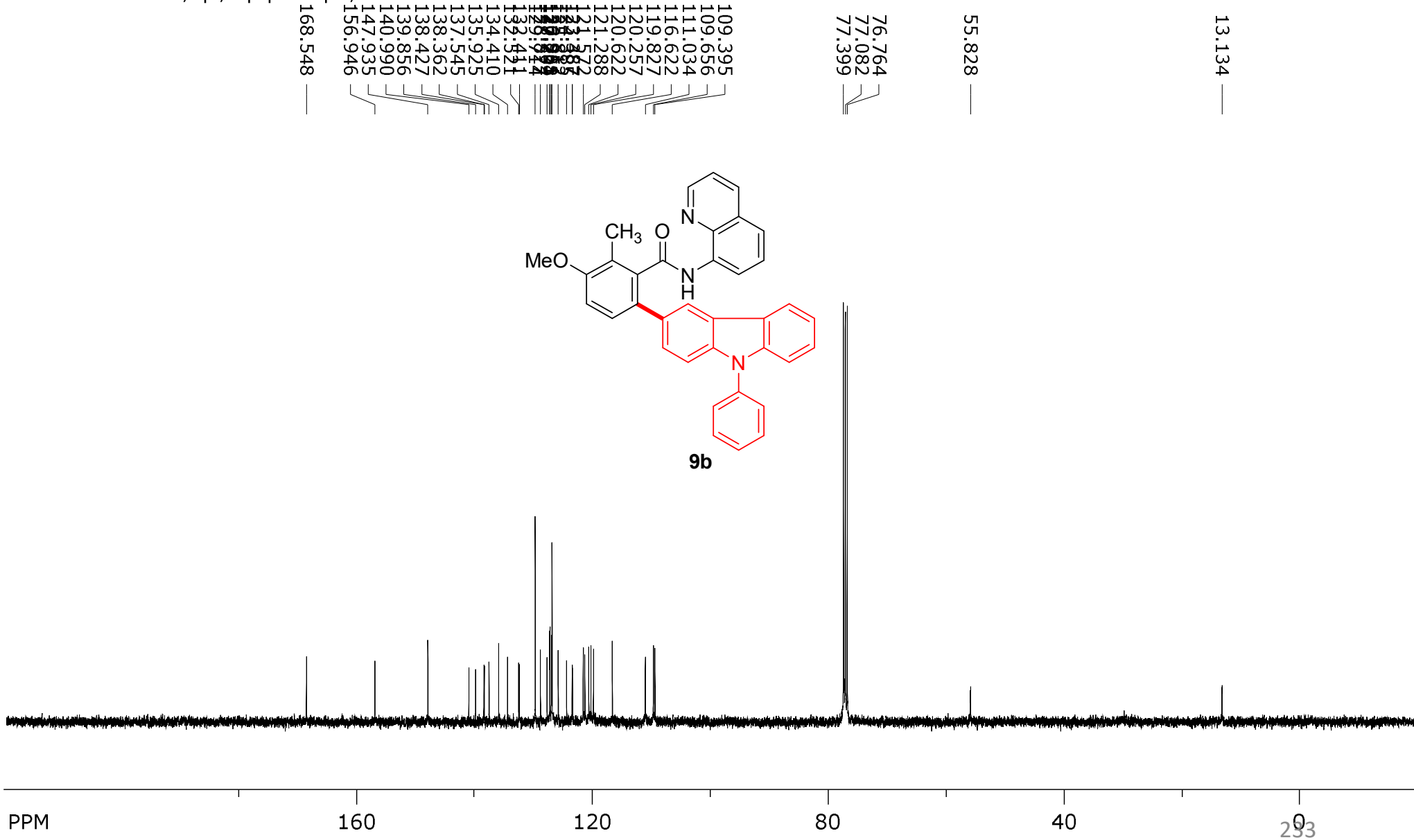
7.0113	—
7.0325	—
7.1522	—
7.1619	—
7.1672	—
7.1732	—
7.1828	—
7.1990	—
7.2361	—
7.2869	—
7.2974	—
7.3156	—
7.3185	—
7.3345	—
7.3540	—
7.3693	—
7.3722	—
7.3851	—
7.3954	—
7.4062	—
7.4148	—
7.4351	—
7.4542	—
7.4739	—
7.4926	—
7.5128	—
7.5171	—
7.5341	—
7.5384	—



SpinWorks 4: RD-946
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

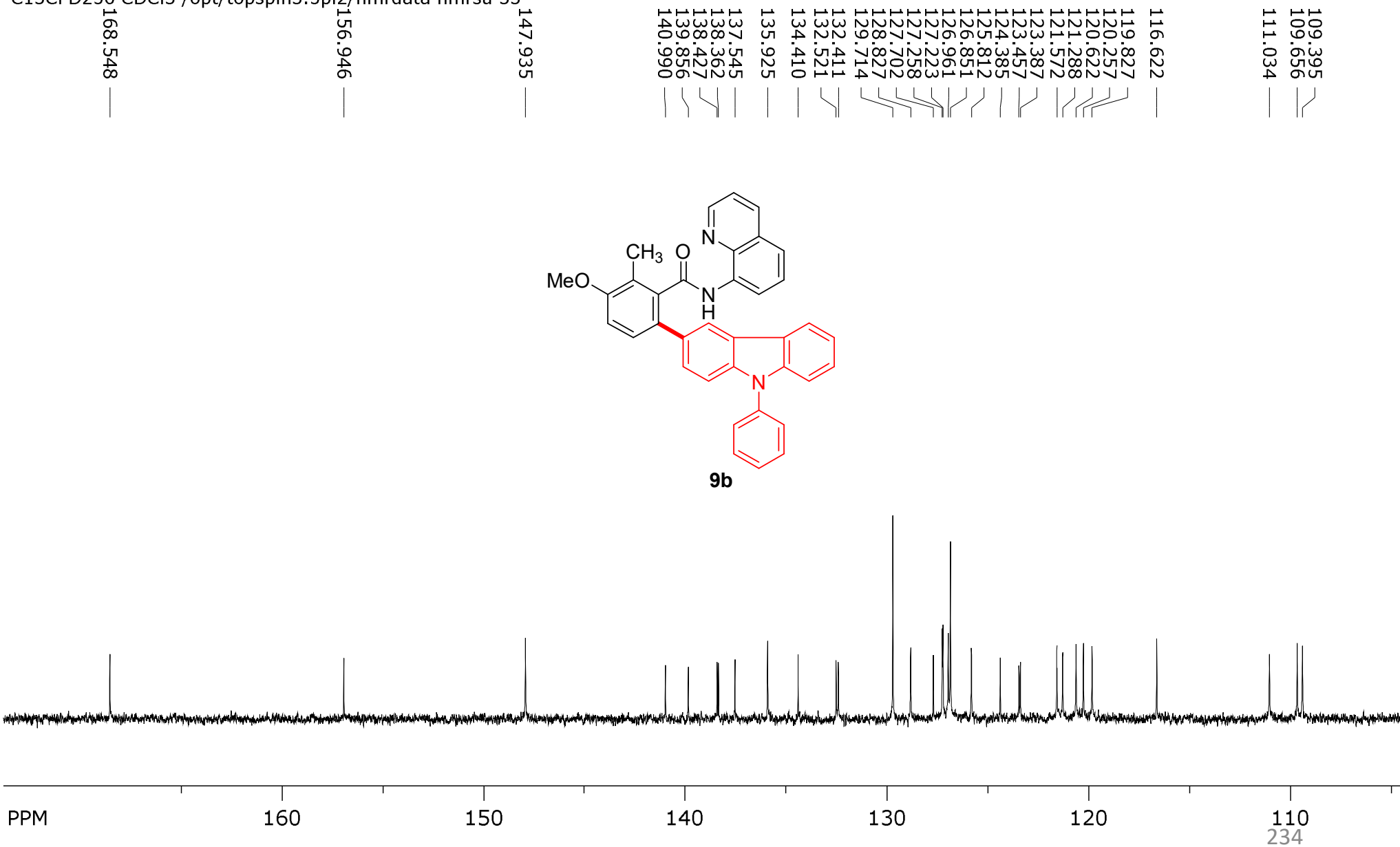


SpinWorks 4: RD-946
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33



SpinWorks 4: RD-946

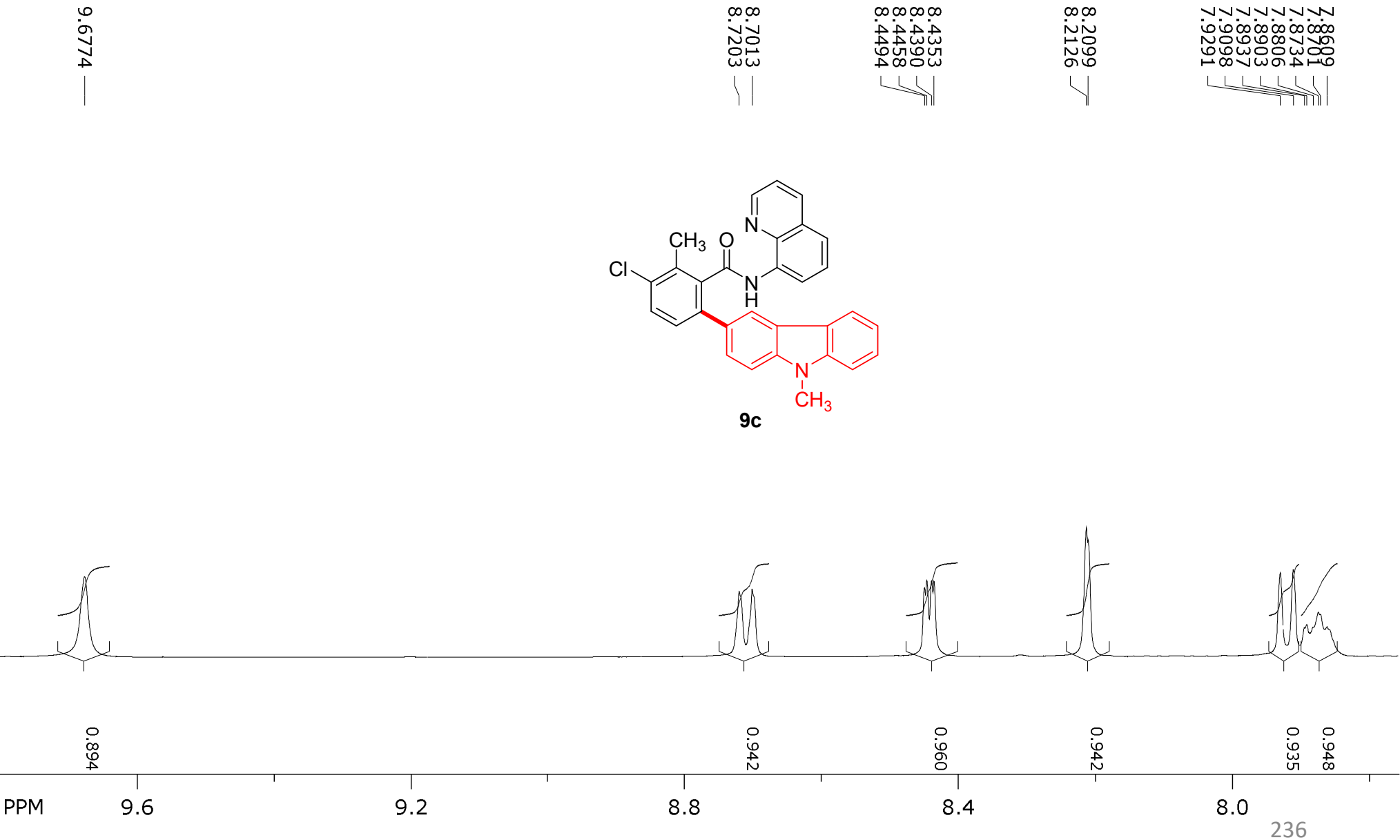
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20



SpinWorks 4: RD 988
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20



SpinWorks 4: RD 988

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

7.5728
7.5771
7.5939
7.5982

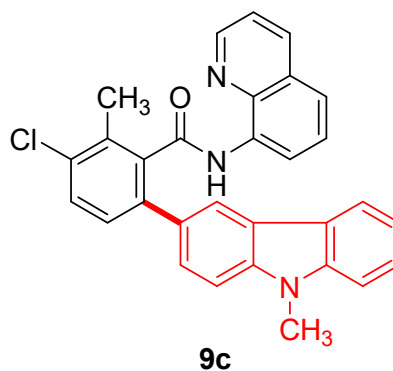
7.5205
7.4998

7.3817
7.4001
7.4023
7.3613
7.3537
7.3463
7.3436
7.3329

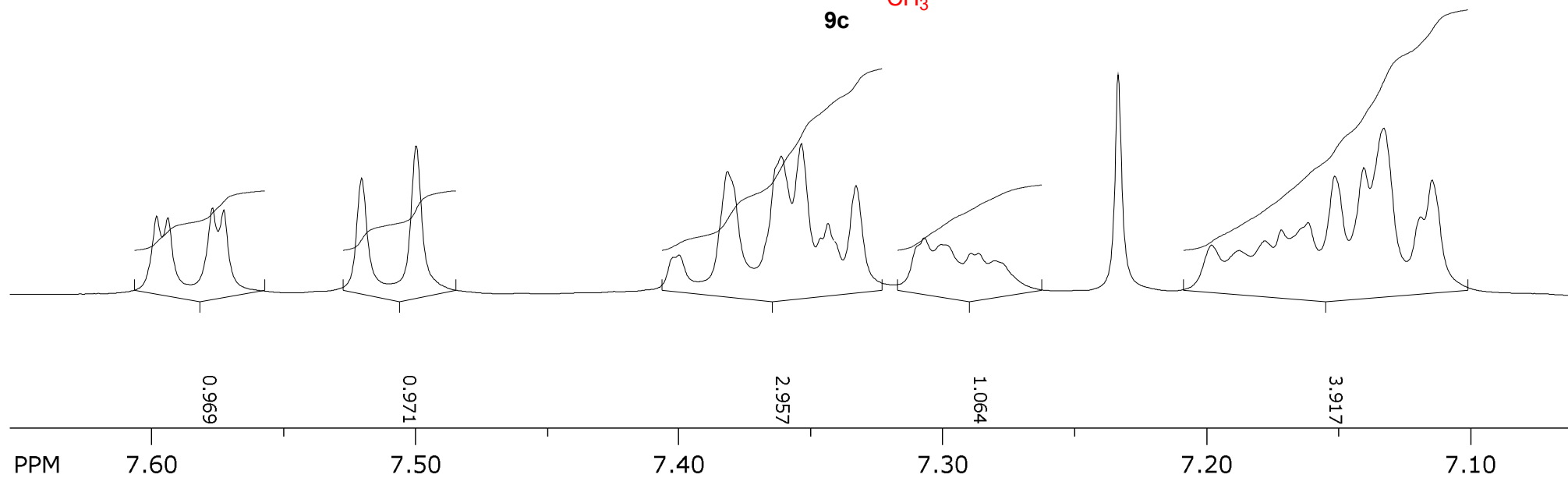
7.3070
7.3006
7.2893
7.2865
7.2803

7.2335

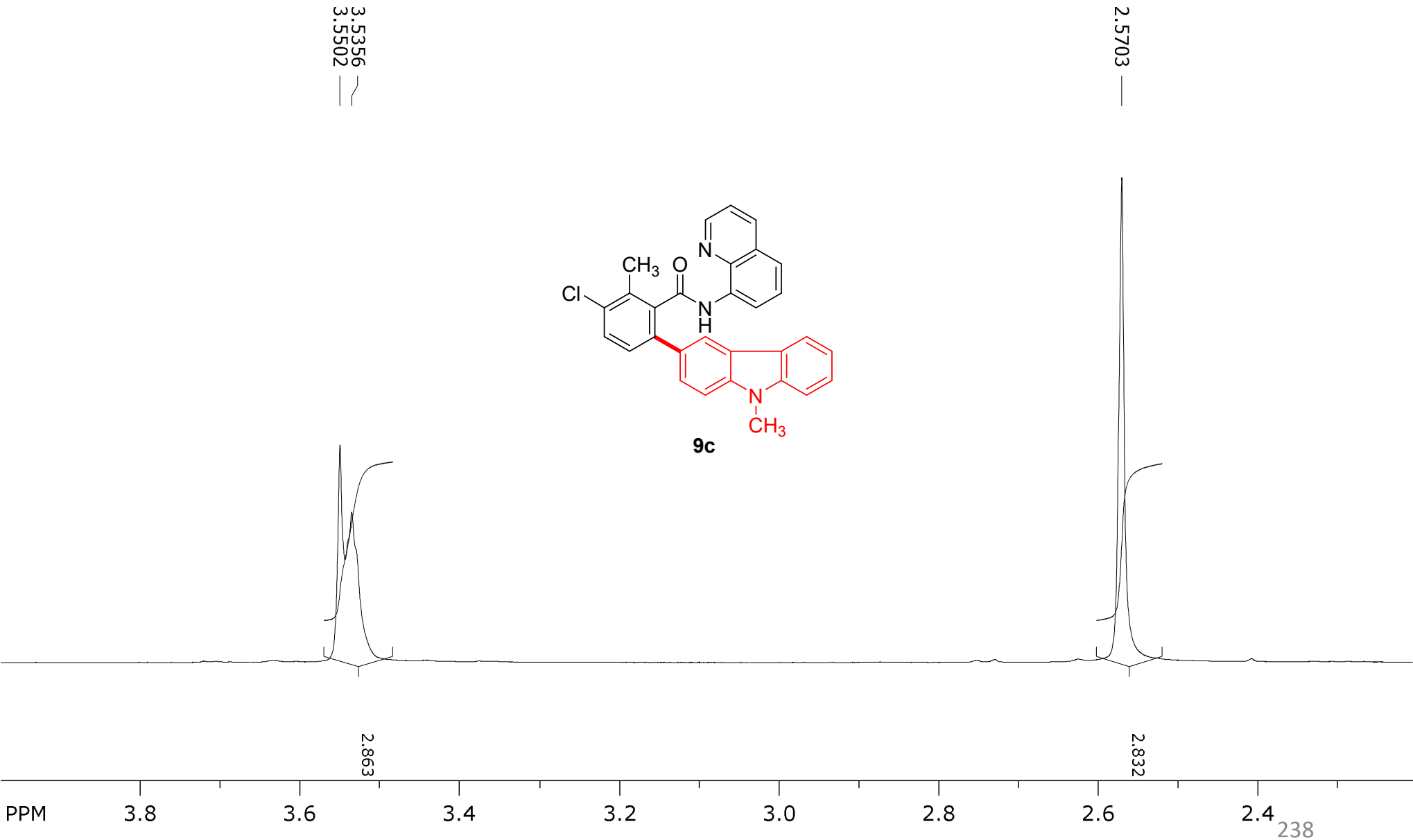
7.1981
7.1876
7.1778
7.1716
7.1615
7.1514
7.1403
7.1327
7.1187
7.1144



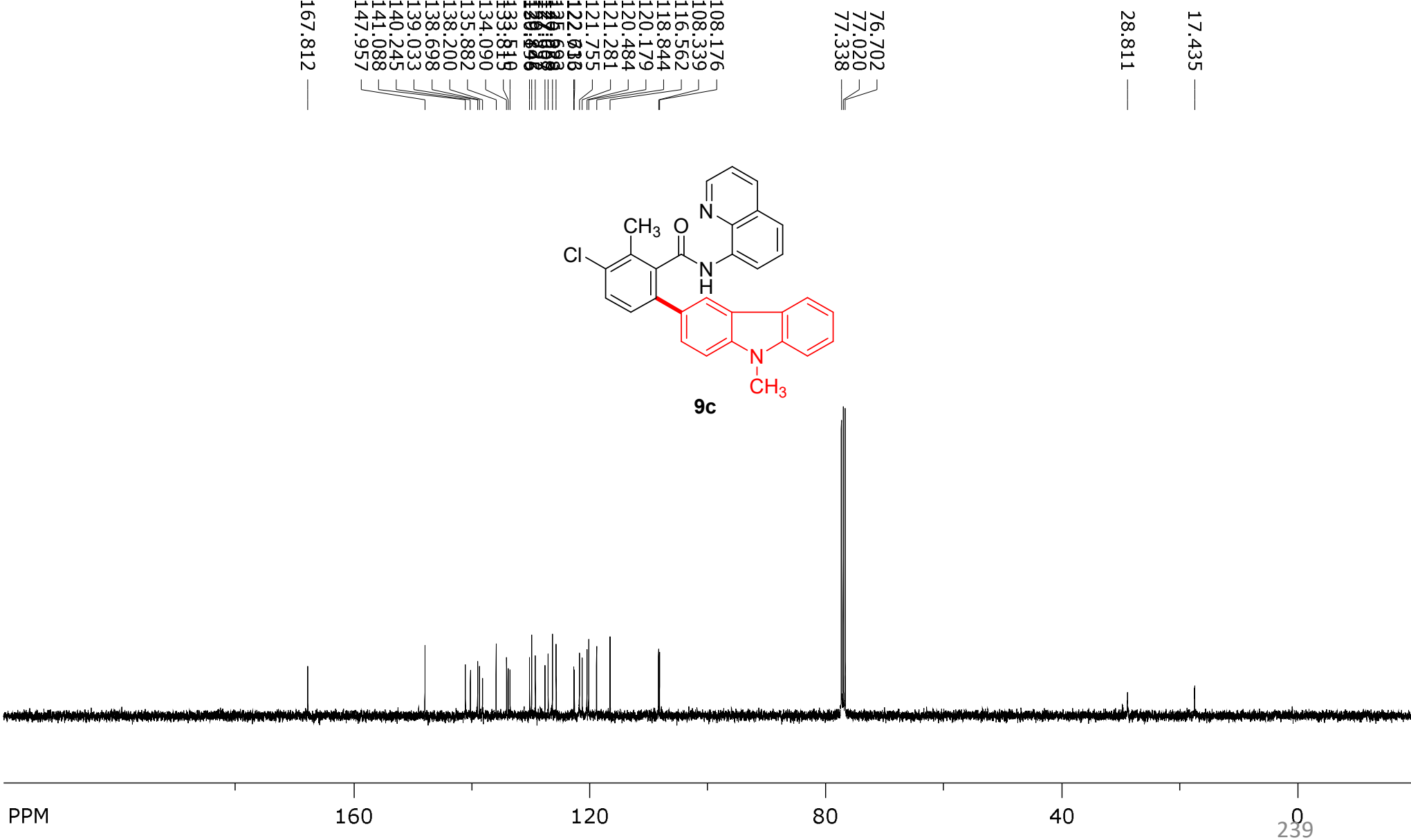
9c



SpinWorks 4: RD 988
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

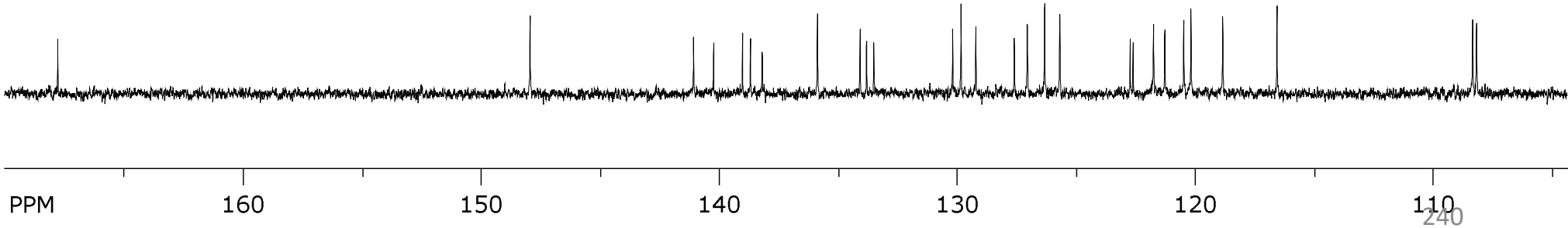
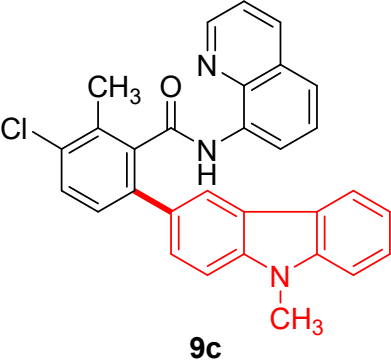


SpinWorks 4: RD 988
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

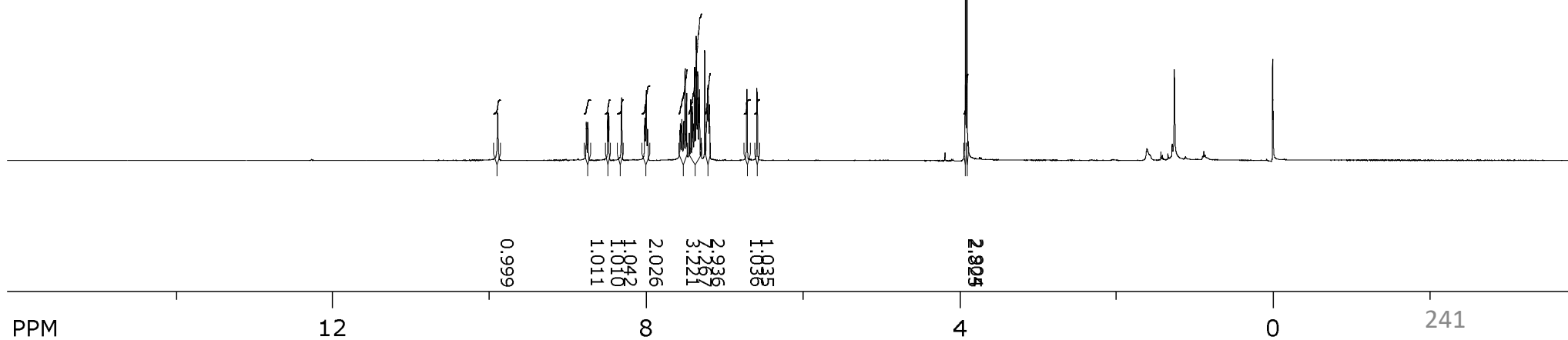
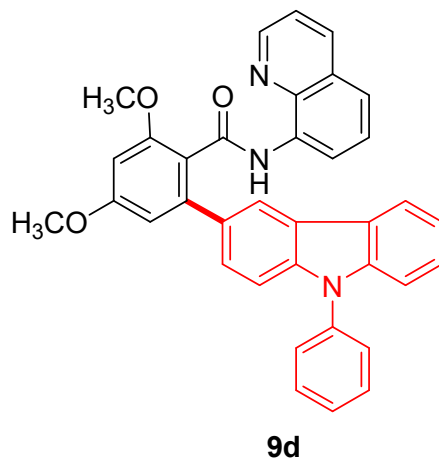
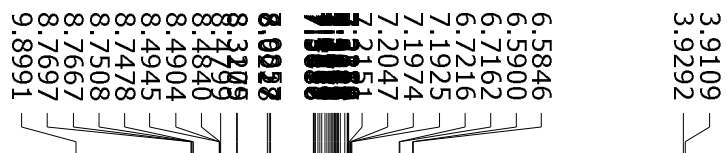


SpinWorks 4: RD 988
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

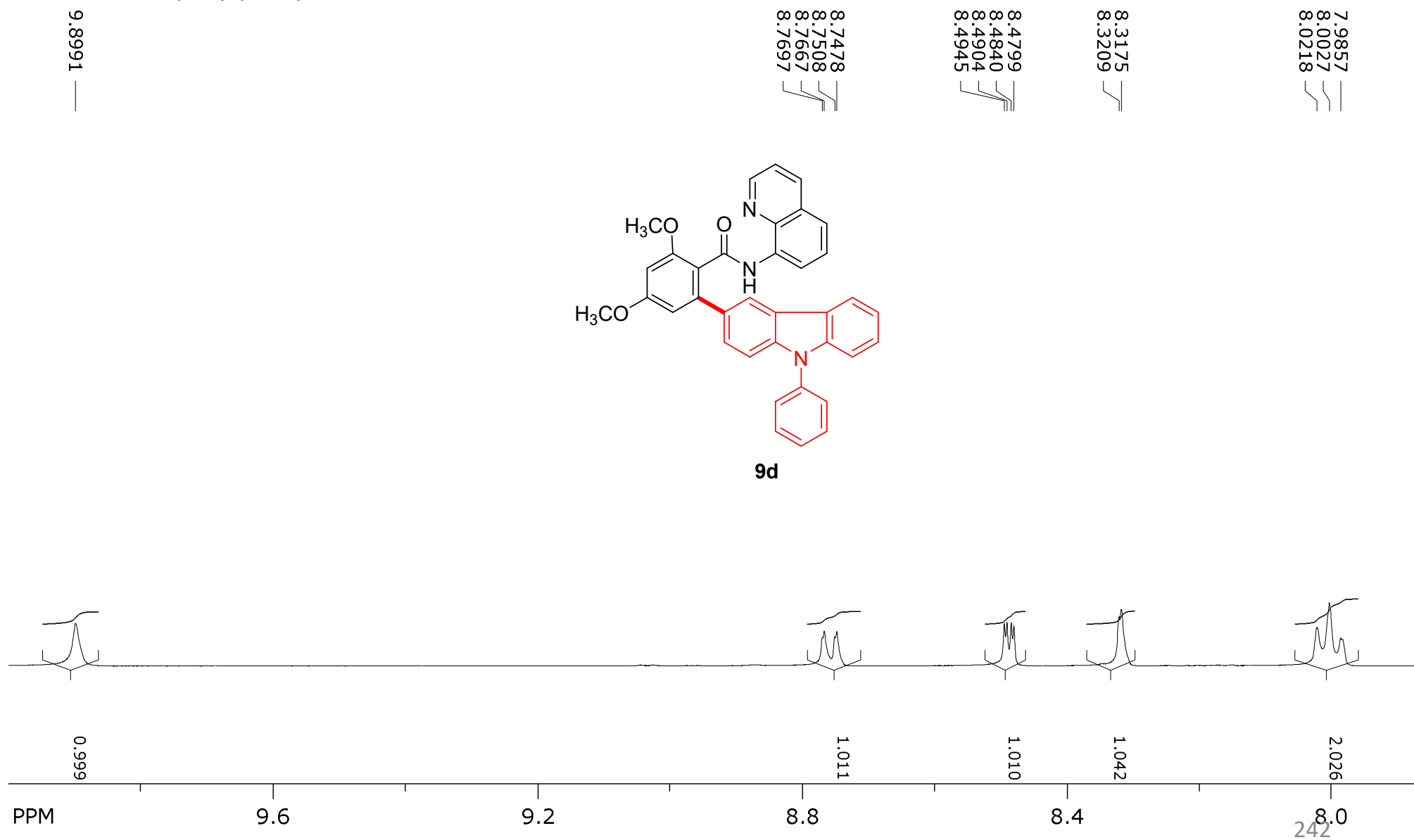
167.812 —
147.957 —
138.200 —
138.698 —
139.033 —
140.245 —
141.088 —
135.882 —
133.815 —
133.510 —
130.196 —
129.845 —
129.222 —
127.607 —
127.058 —
126.328 —
125.693 —
122.736 —
122.613 —
121.755 —
121.281 —
120.484 —
120.179 —
118.844 —
116.562 —
108.339 —
108.176 —



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

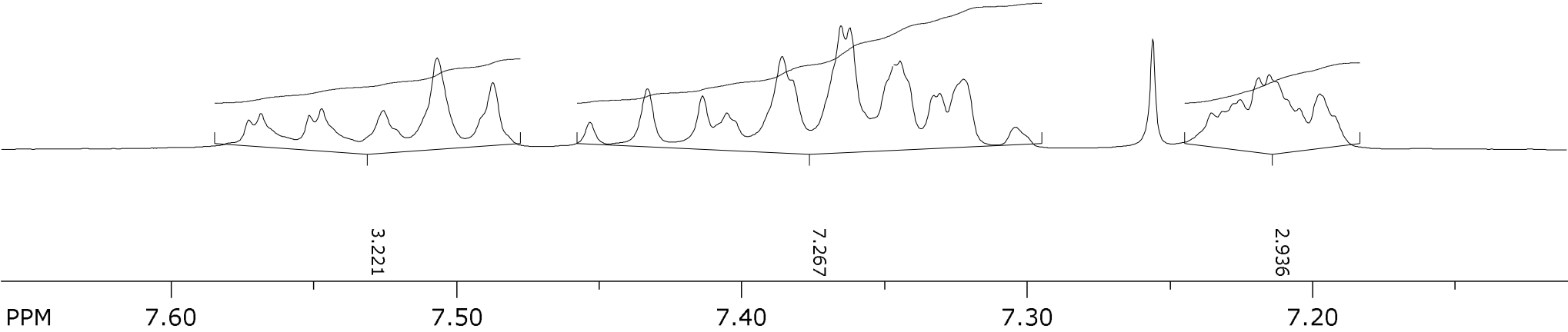
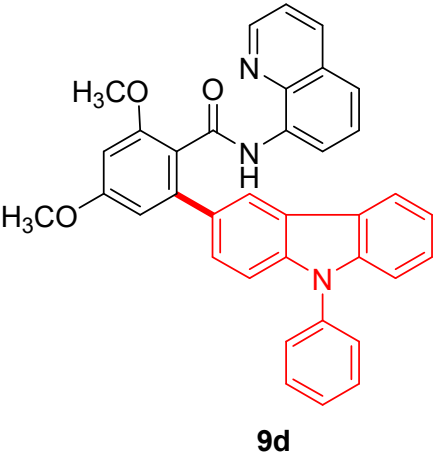


SpinWorks 4: RD-949
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



SpinWorks 4: RD-949
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

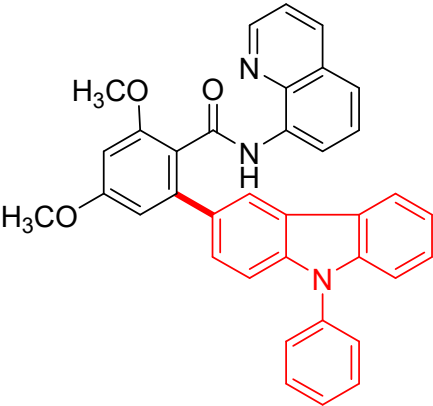
7.1925
7.1974
7.2047
7.2151
7.2189
7.2253
7.2275
7.2315
7.2354
7.2559
7.3046
7.3222
7.3306
7.3327
7.3445
7.3465
7.3622
7.3653
7.3825
7.3859
7.4053
7.4138
7.4331
7.4515
7.5069
7.5257
7.5473
7.5517
7.5686



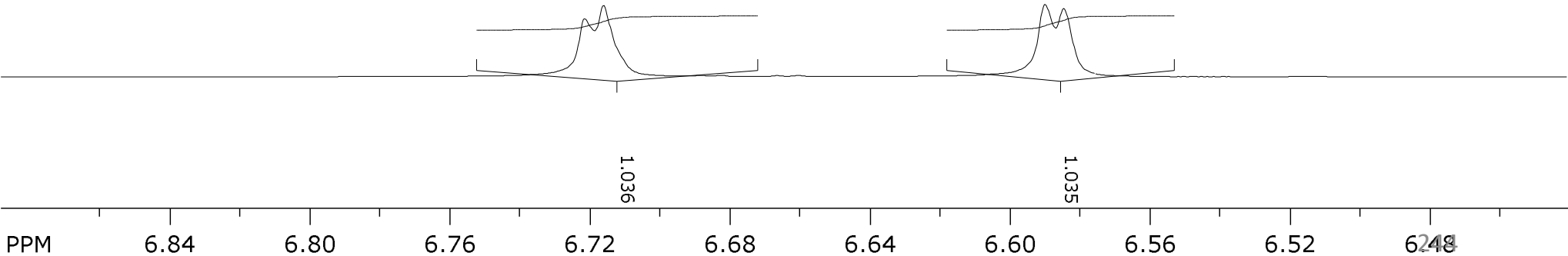
SpinWorks 4: RD-949
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

6.7162
6.7216

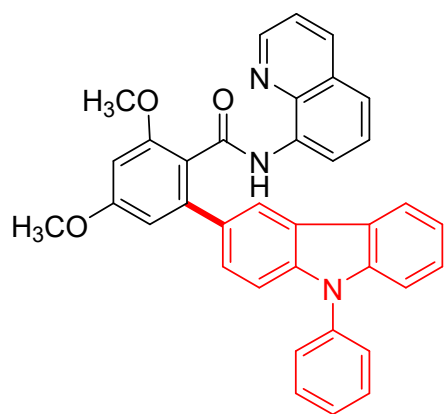
6.5846
6.5900



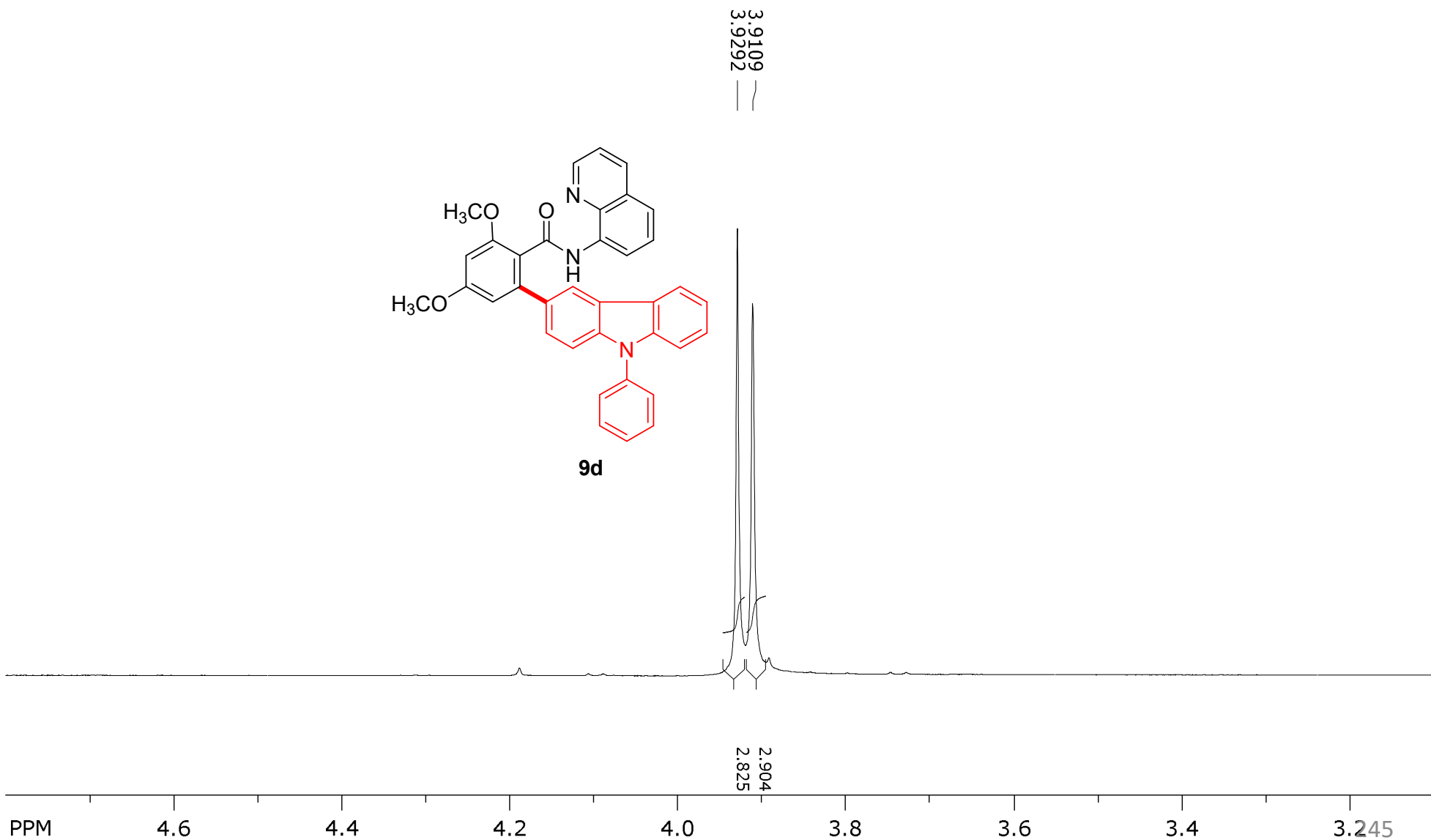
9d



SpinWorks 4: RD-949
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27



9d

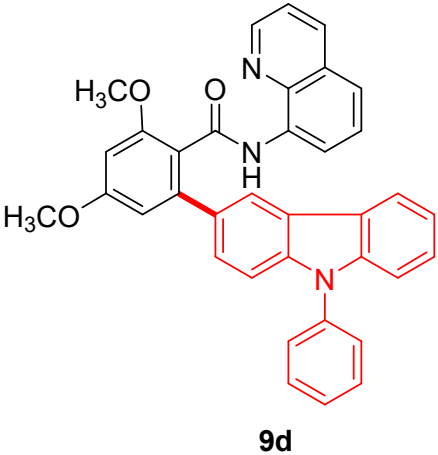


SpinWorks 4: RD 949
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 15

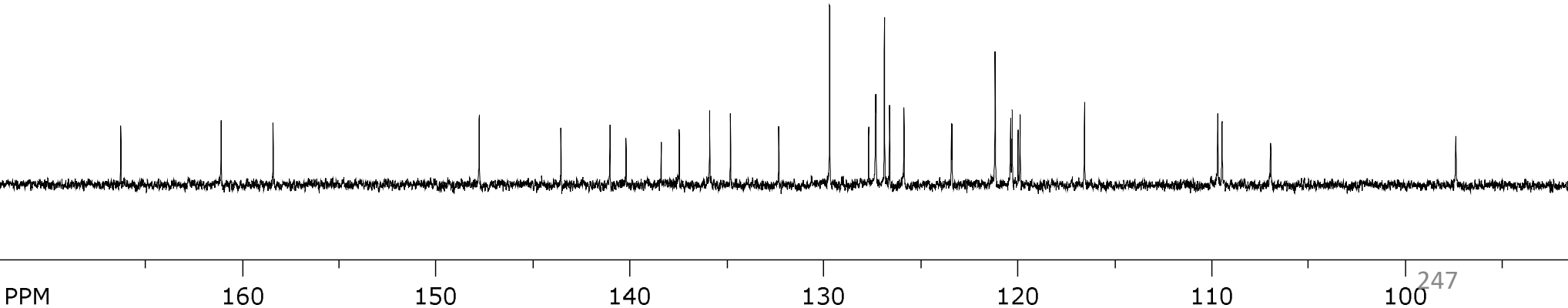
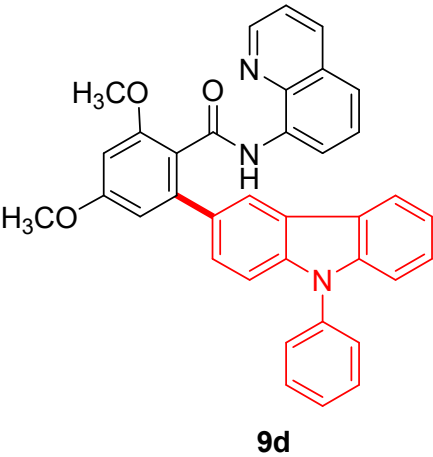
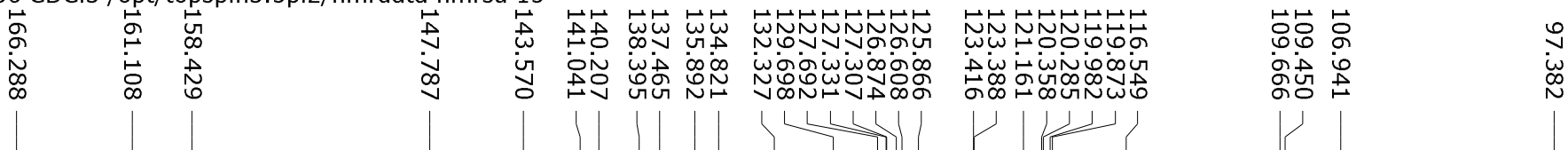
97.382
106.941
109.450
109.666
116.549
119.873
119.982
120.285
120.358
121.181
121.488
121.865
121.865
129.698
132.327
134.821
135.892
137.465
138.395
140.207
141.041
143.570
147.787
158.429
161.108
166.288

76.702
77.020
77.337

55.581
56.035



SpinWorks 4: RD 949
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 15



Chemical structure of compound **11a** is shown above the spectrum. The structure is a complex molecule featuring a central benzene ring substituted with a furan ring, a quinoline ring, and a dimethylcarbamate group.

The ¹H NMR spectrum (400 MHz, CDCl₃) displays the following peaks (ppm) and integrations:

Peak (ppm)	Integration
1.7526	9.163
1.078	1.078
1.123	1.123
1.127	1.127
1.131	1.131
1.139	1.139
2.263	2.263
2.216	2.216
7.9339	1.139
8.1832	2.263
8.3166	1.131
8.3381	1.131
8.3498	1.131
8.3708	1.131
8.7985	1.131
8.8178	1.131
10.1028	1.000



248

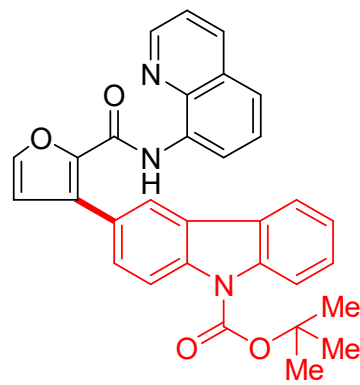
SpinWorks 4: RD-363-RE
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

8.7985
8.8178

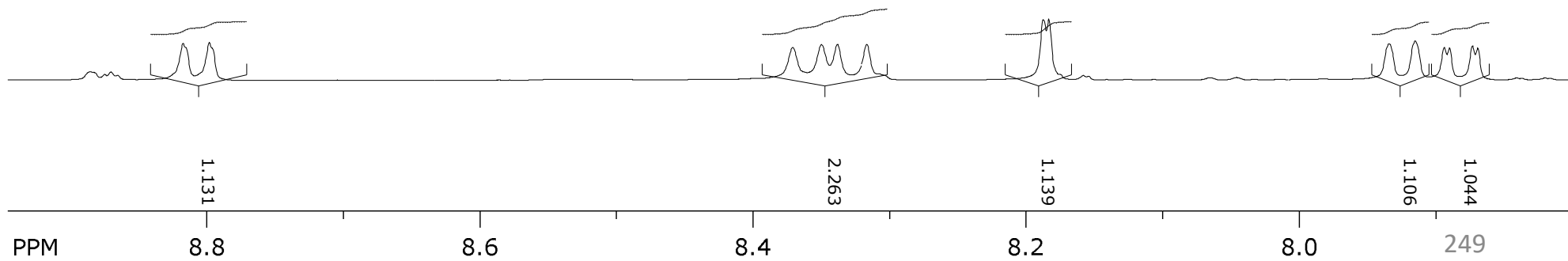
8.3166
8.3381
8.3498
8.3708

8.1832
8.1874

7.8687
7.8726
7.8894
7.8933
7.9147
7.9339

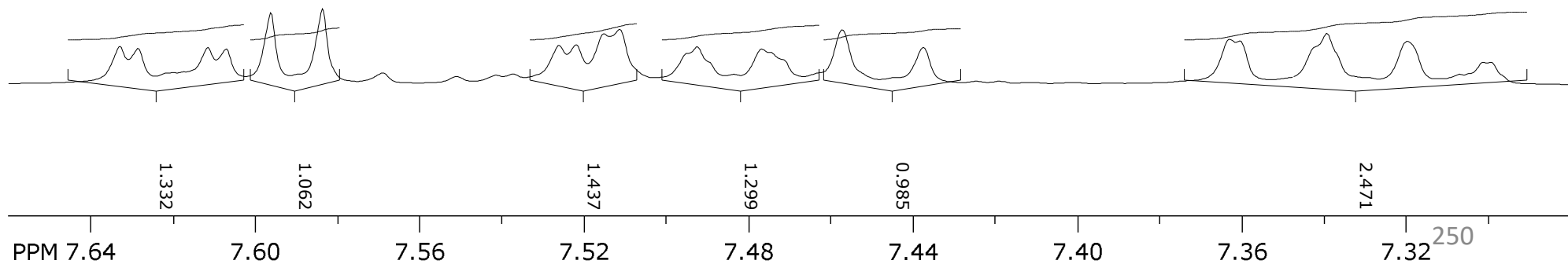
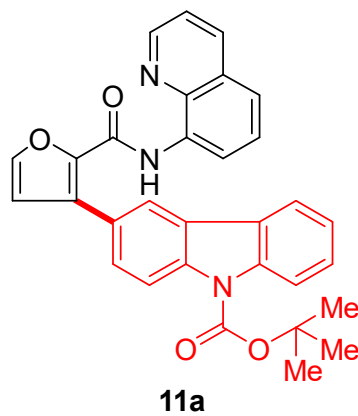


11a



SpinWorks 4: RD-363-RE
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

7.6287	7.5838	7.5115	7.4926	7.4748	7.4573	7.4376	7.3606	7.3393	7.3198	7.3012
7.6331	7.6073	7.5154	7.4948	7.4769	—	—	7.3631	—	—	—
—	—	—	—	—	—	—	—	—	—	—



SpinWorks 4: RD-363-RE
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

7.3606
7.3631

7.3393

7.3198

7.3012

7.2532

7.1961

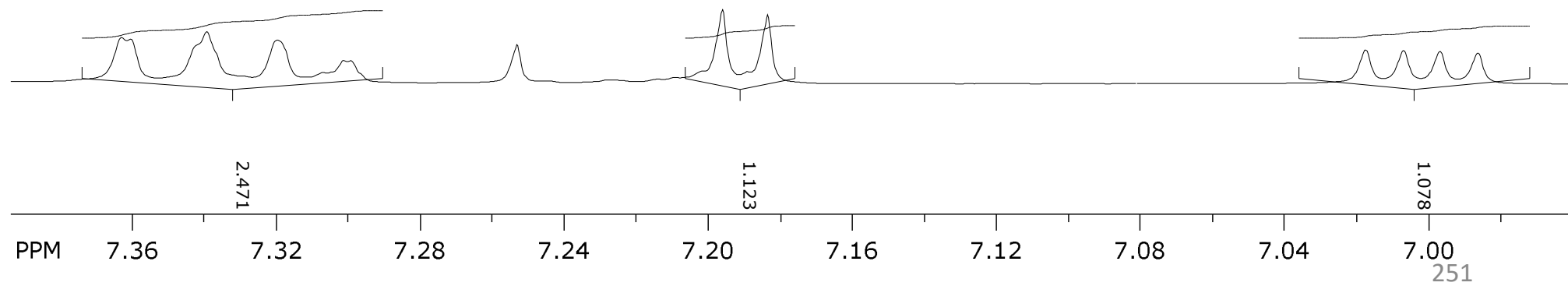
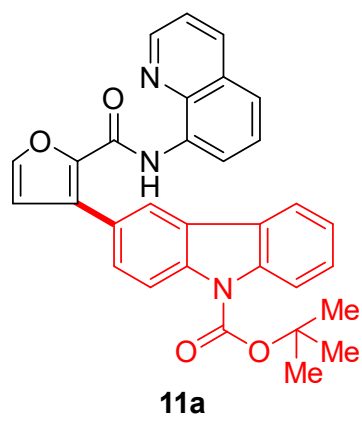
7.1836

7.0175

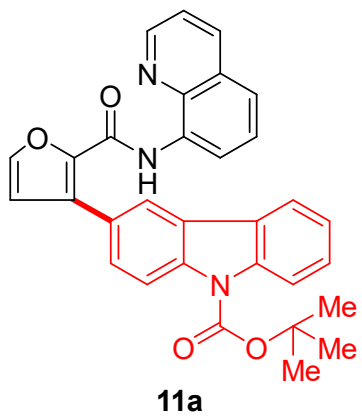
7.0069

6.9968

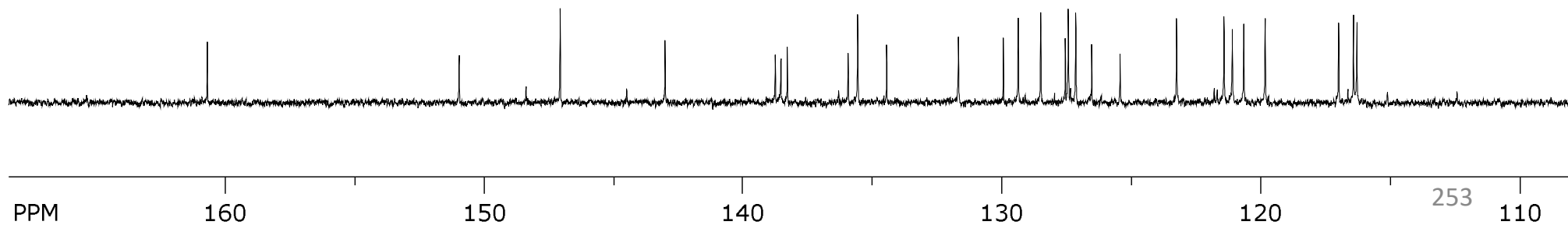
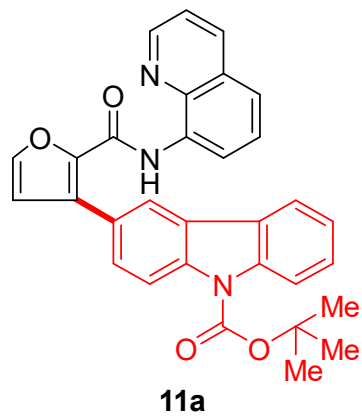
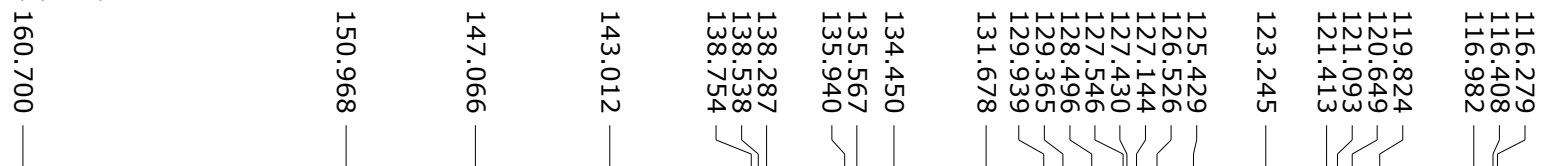
6.9863



SpinWorks 4: RD-363-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



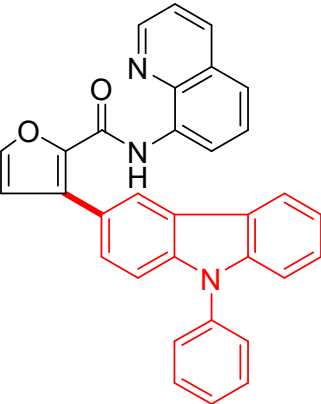
SpinWorks 4: RD-363-RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



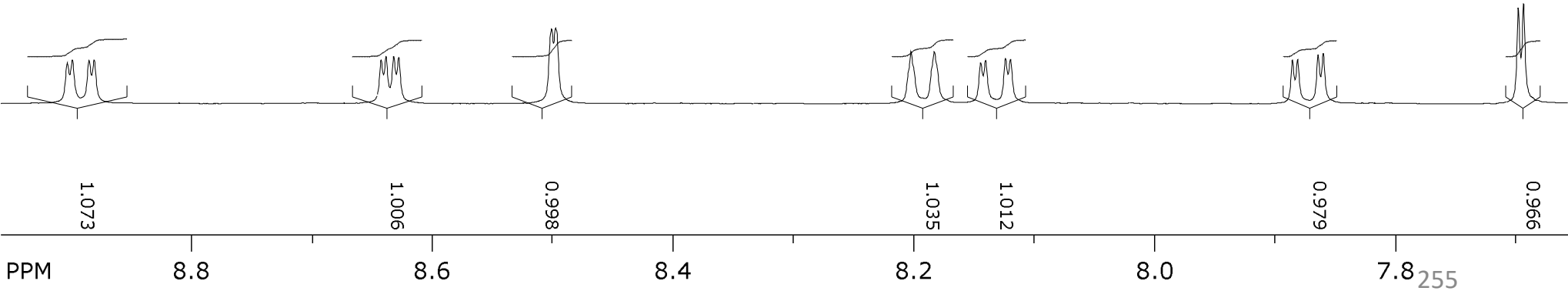
PPM



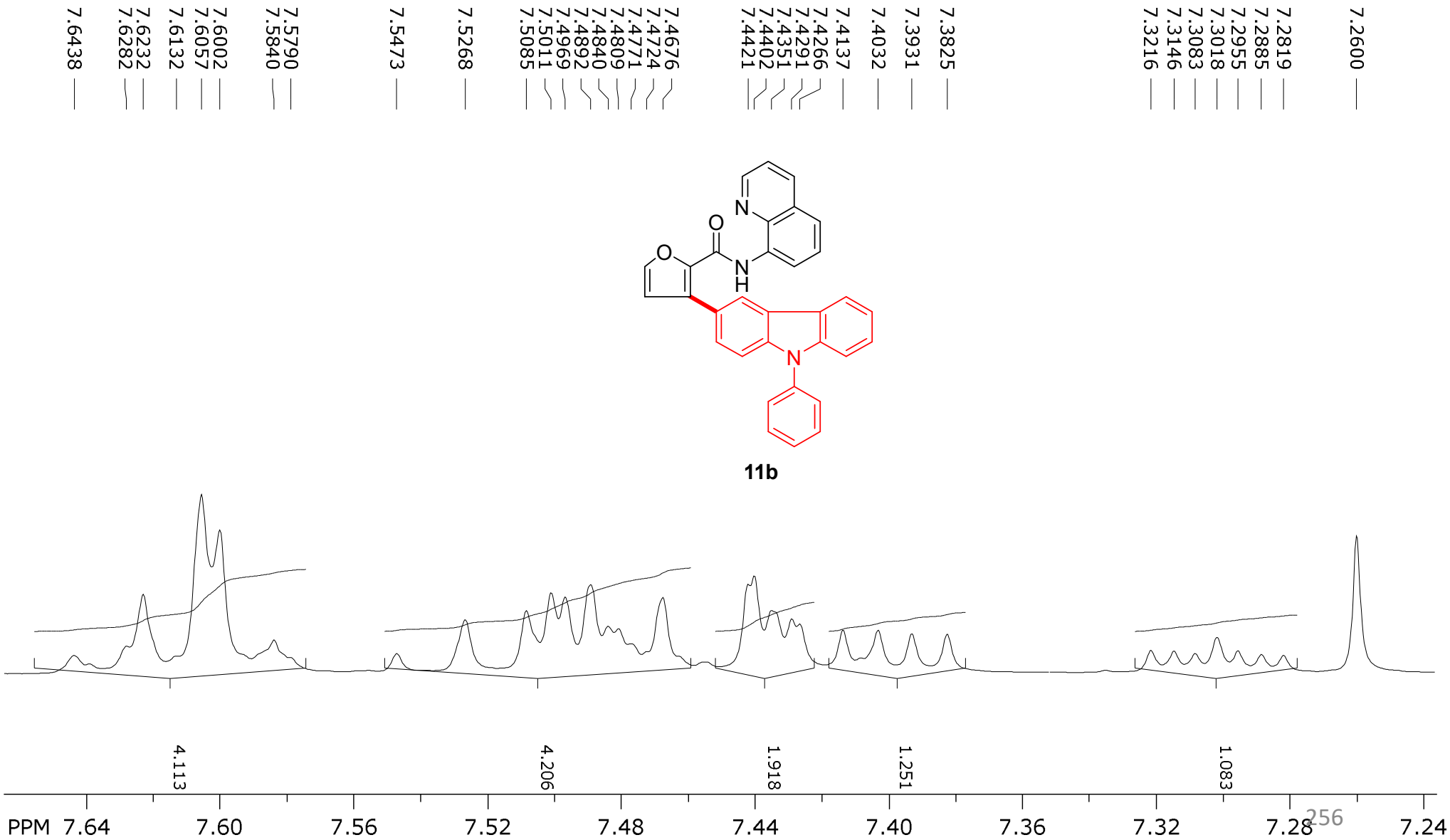
SpinWorks 4: RD-218-rep 1



11b

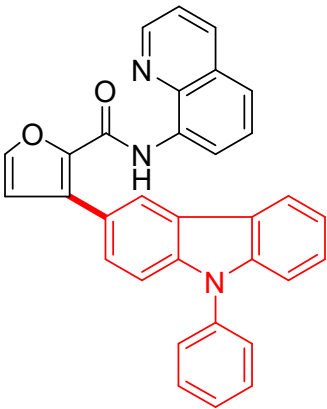


SpinWorks 4: RD-218-rep 1



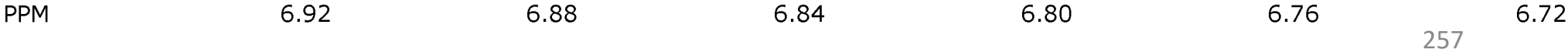
SpinWorks 4: RD-218-rep 1

6.8263
6.8306

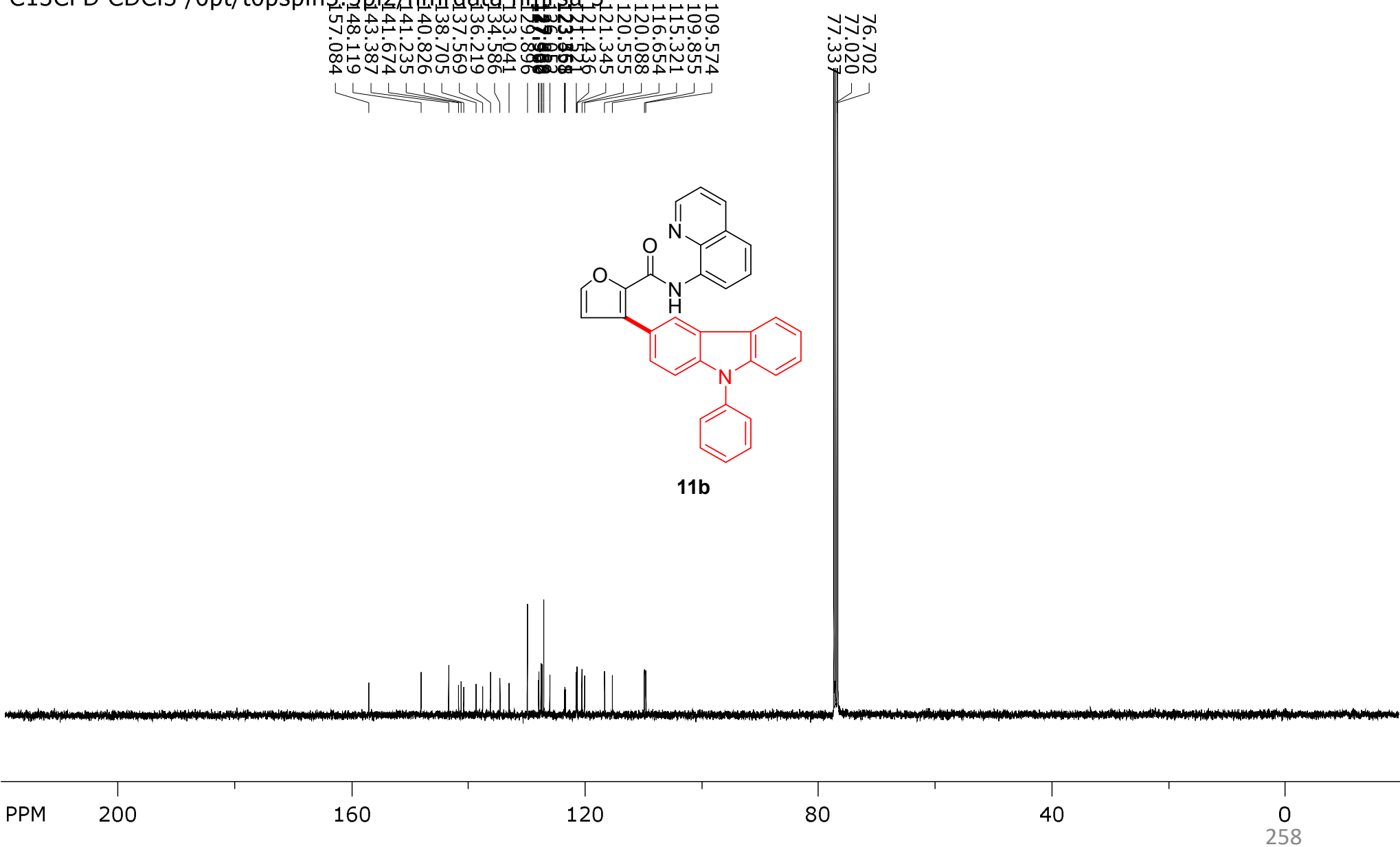


11b

0.958

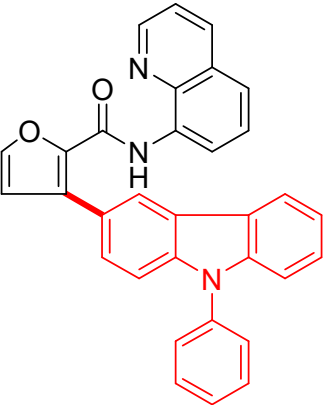


SpinWorks 4: RD 218 REP1
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

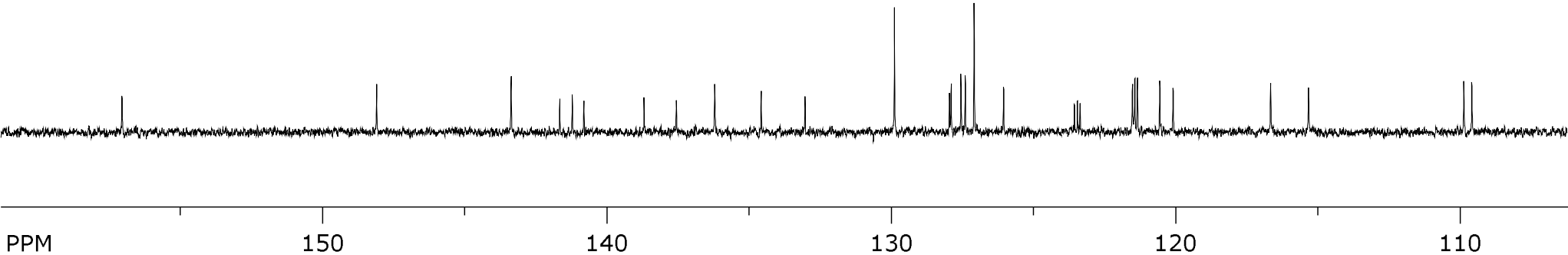


SpinWorks 4: RD 218 REP1
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata_nmr su 3

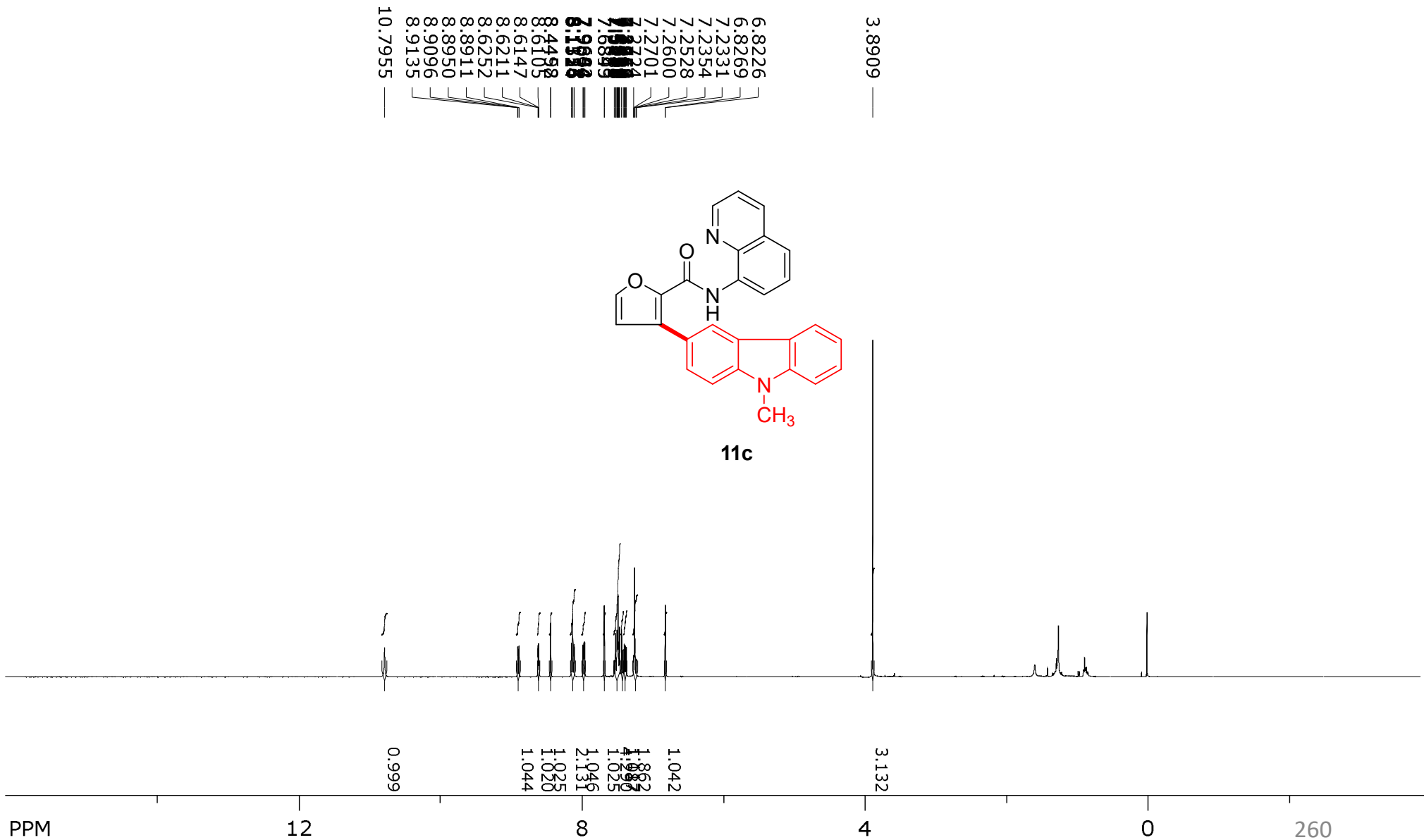
157.084 —
148.119 —
143.387 —
141.674 —
140.826 —
141.235 —
138.705 —
137.569 —
136.219 —
134.586 —
133.041 —
129.896 —
127.900 —
127.556 —
127.402 —
127.089 —
126.052 —
123.558 —
123.455 —
123.361 —
121.521 —
121.436 —
121.345 —
120.555 —
120.088 —
116.654 —
115.321 —
109.855 —
109.574 —



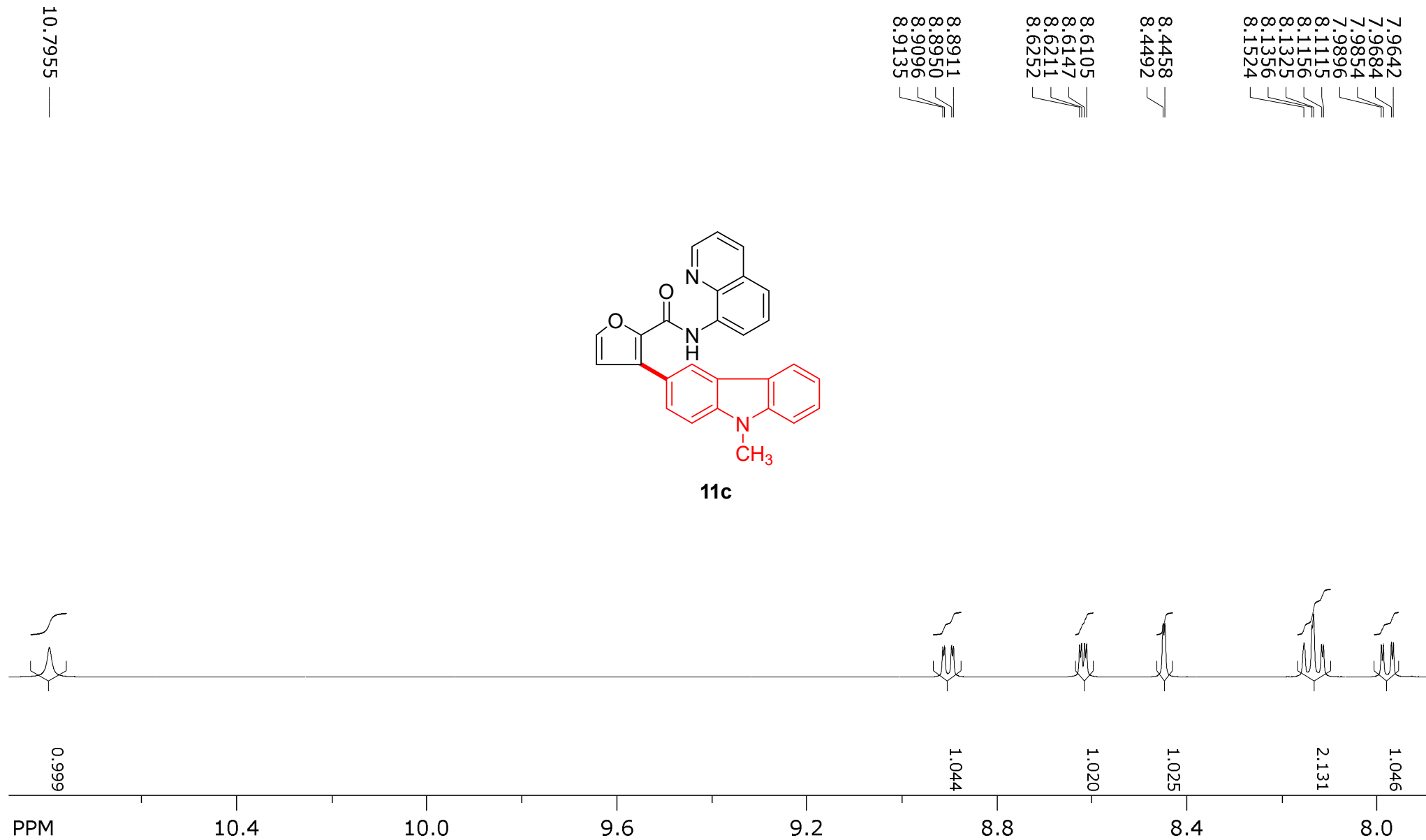
11b



SpinWorks 4: rd-300



SpinWorks 4: rd-300

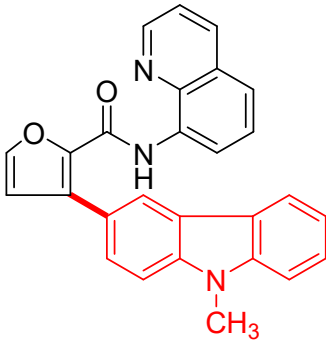


SpinWorks 4: rd-300

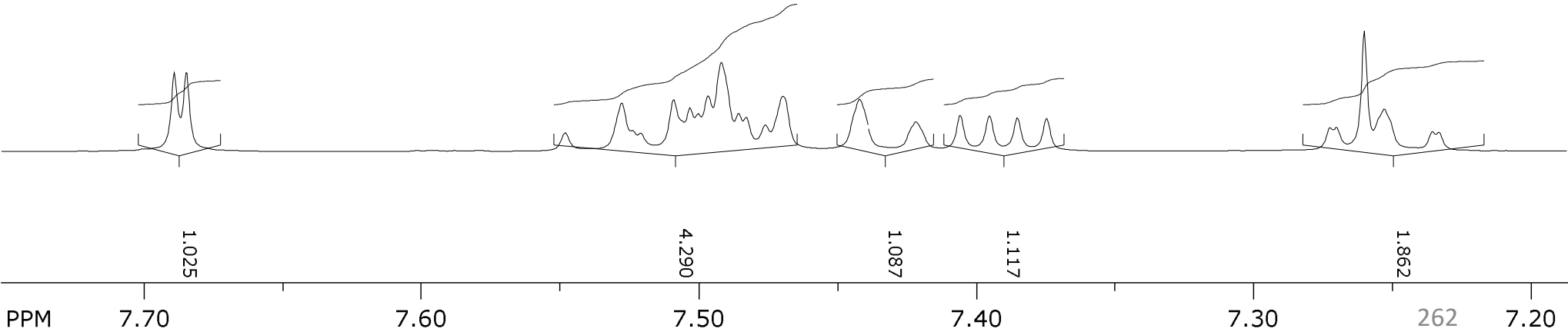
7.6849
7.6893

7.5482
7.5278
7.5240
7.5210
7.5091
7.5032
7.5003
7.4967
7.4919
7.4857
7.4829
7.4760
7.4696
7.4421
7.4217
7.4058
7.3952
7.3852
7.3746

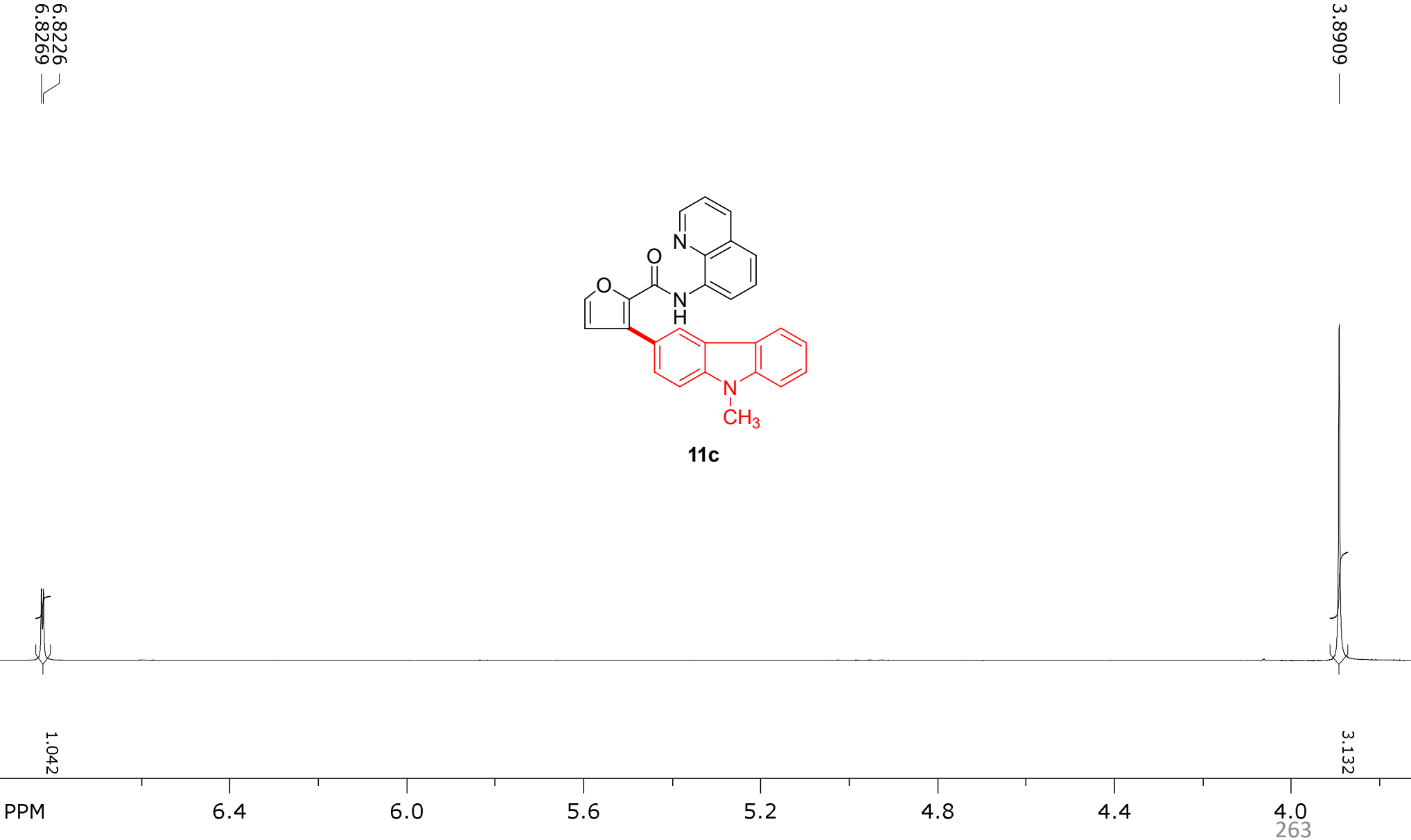
7.2724
7.2701
7.2600
7.2528
7.2354
7.2331

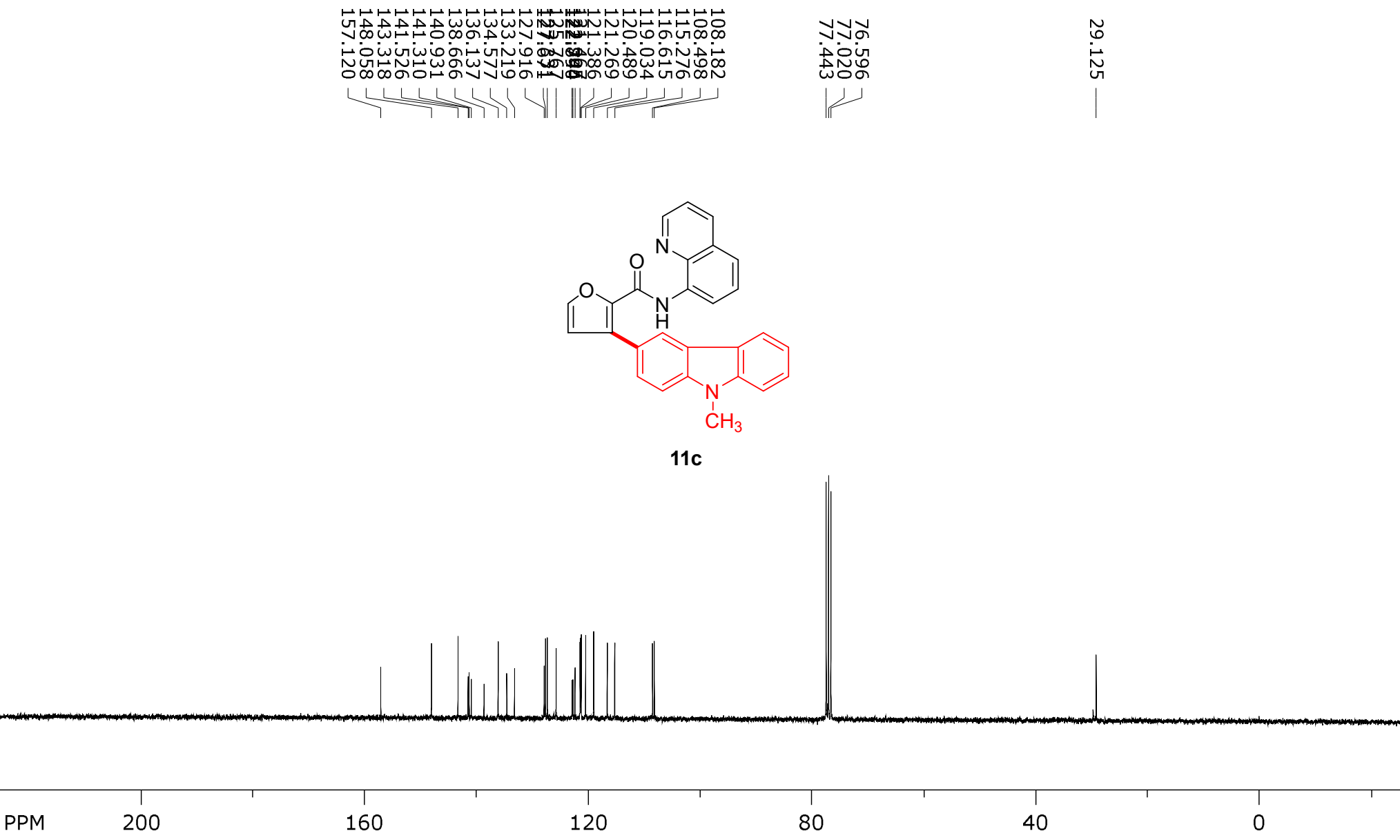


11c



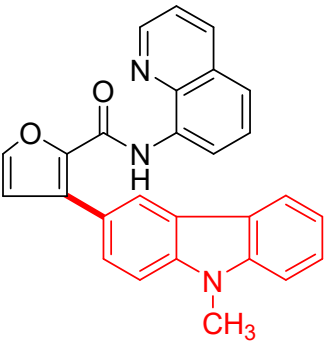
SpinWorks 4: rd-300





SpinWorks 4: SAB-26

157.120 —
148.058 —
143.318 —
141.310 —
140.931 —
138.666 —
136.137 —
134.577 —
133.219 —
127.916 —
127.671 —
127.331 —
125.767 —
122.890 —
122.744 —
122.395 —
121.467 —
121.386 —
121.269 —
120.489 —
119.034 —
116.615 —
115.276 —
108.498 —
108.182 —



11c



PPM

150

140

130

120

110

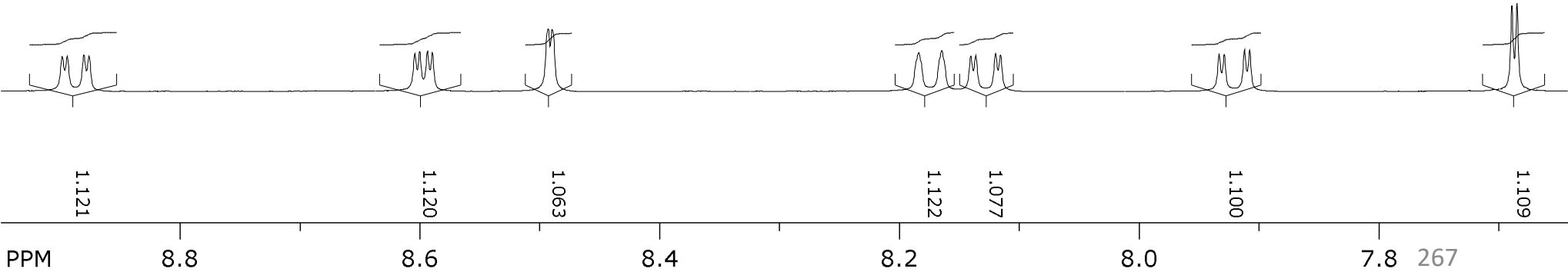
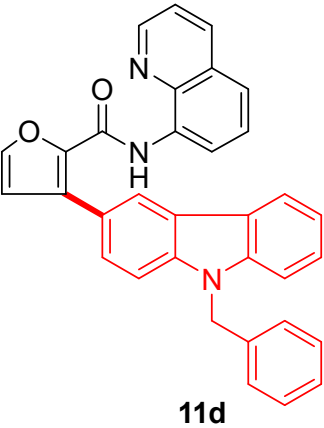
265

PPM



11d

SpinWorks 4: rd-315



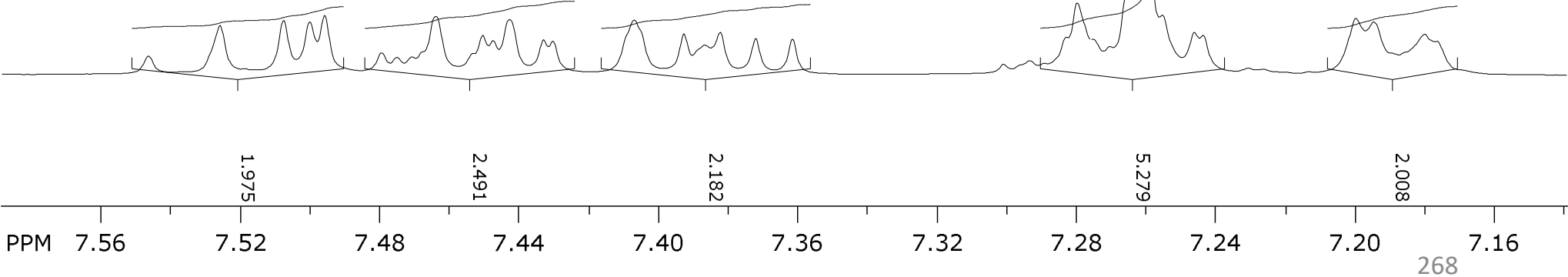
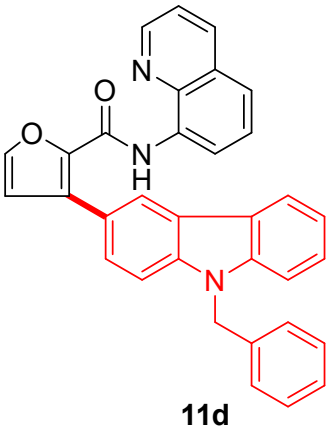
SpinWorks 4: rd-315

7.5465 —
7.5259 —
7.5001 —
7.5077 —
7.4959 —
7.4795 —
7.4751 —
7.4708 —
7.4640 —
7.4532 —
7.4505 —
7.4475 —
7.4427 —
7.4330 —
7.4303 —

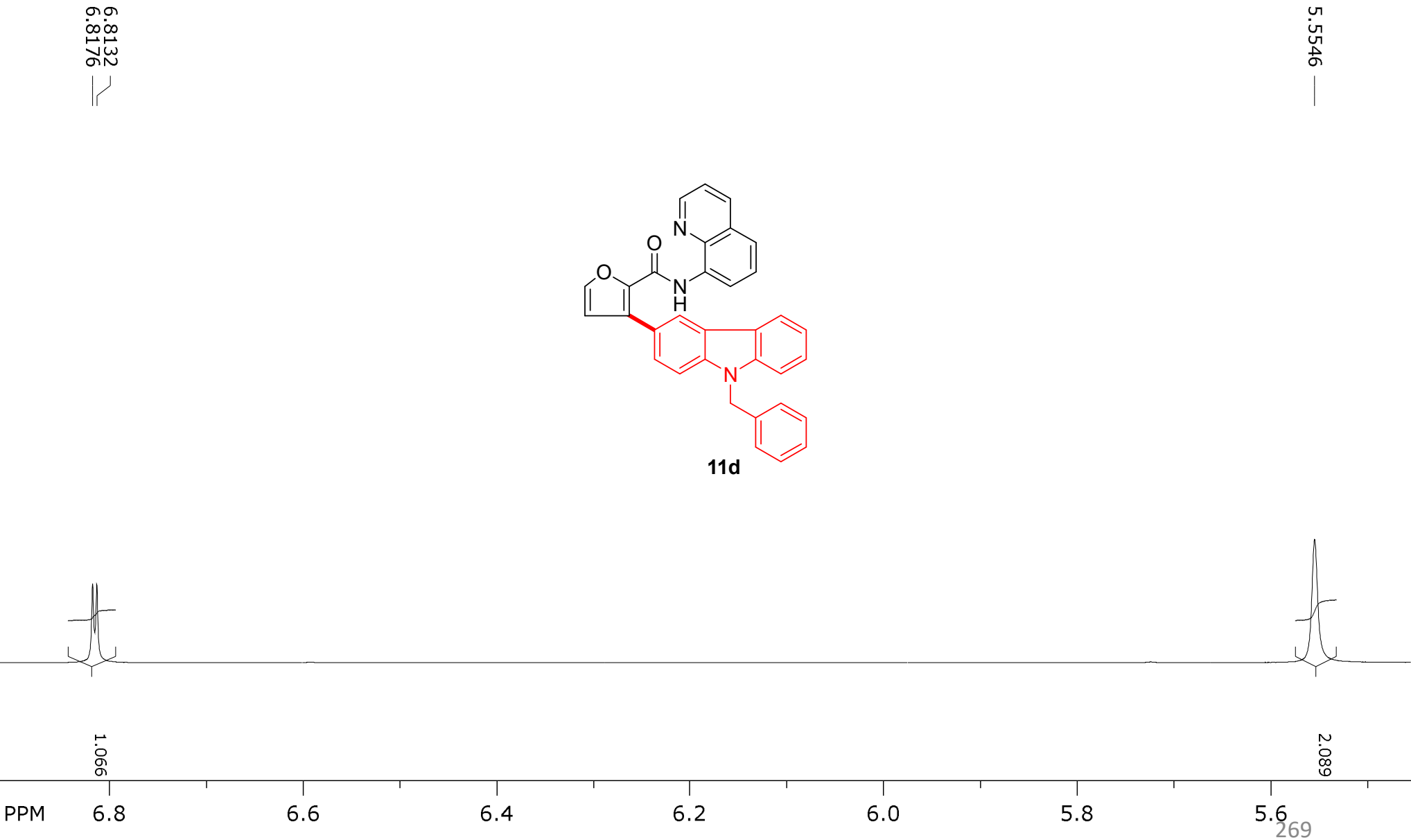
7.4069 —
7.3927 —
7.3867 —
7.3822 —
7.3721 —
7.3615 —

7.2829 —
7.2797 —
7.2751 —
7.2703 —
7.2652 —
7.2600 —
7.2553 —
7.2461 —
7.2436 —

7.1945 —
7.1799 —
7.1764 —

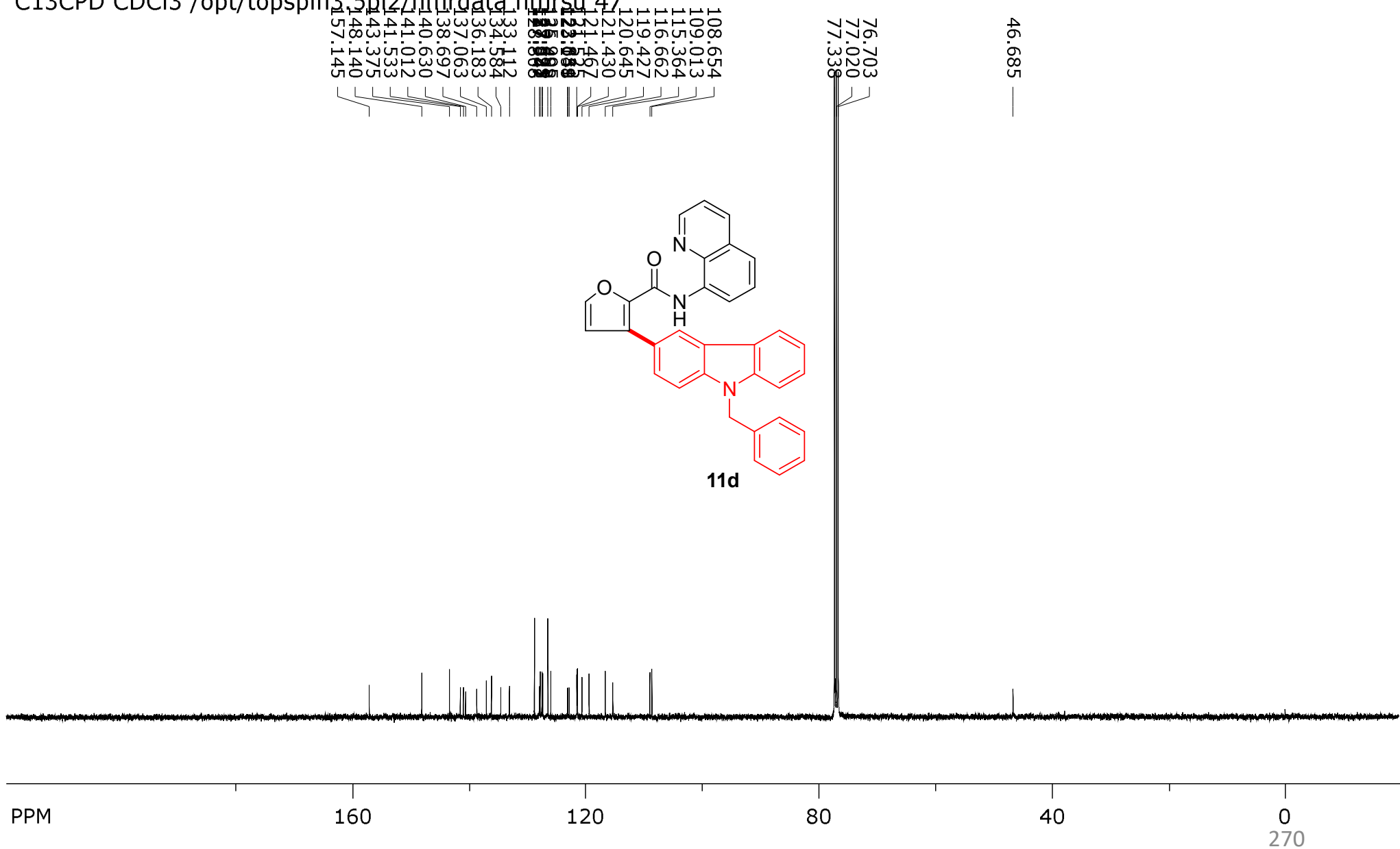
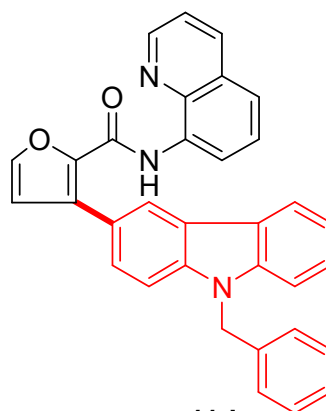


SpinWorks 4: rd-315

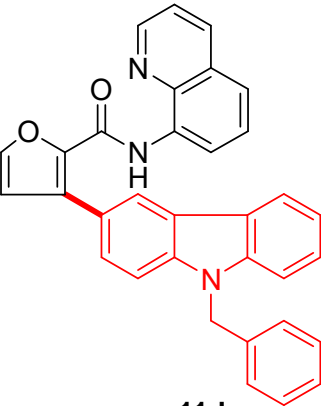
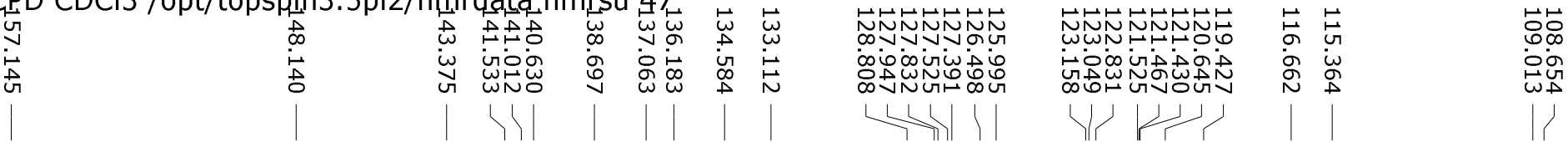


C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata/nmr su_47

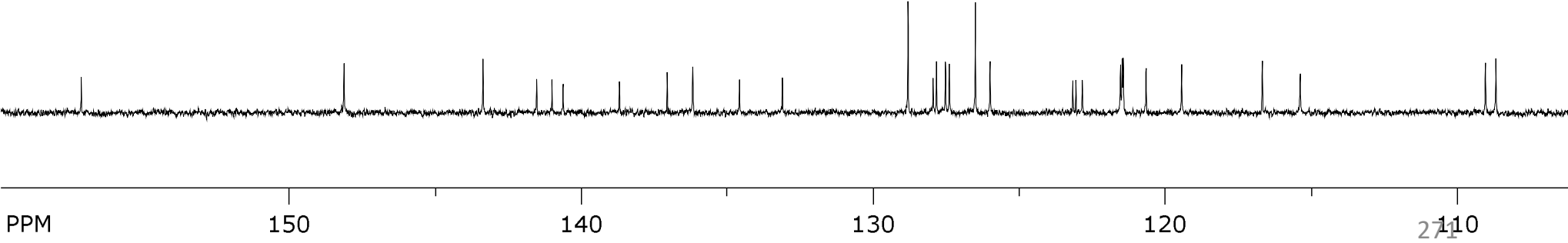
108.654
109.013
115.364
116.662
119.427
120.645
121.430
121.467
122.089
125.088
126.088
133.112
134.584
136.183
137.063
138.697
140.630
141.012
141.533
143.375
148.140
157.145



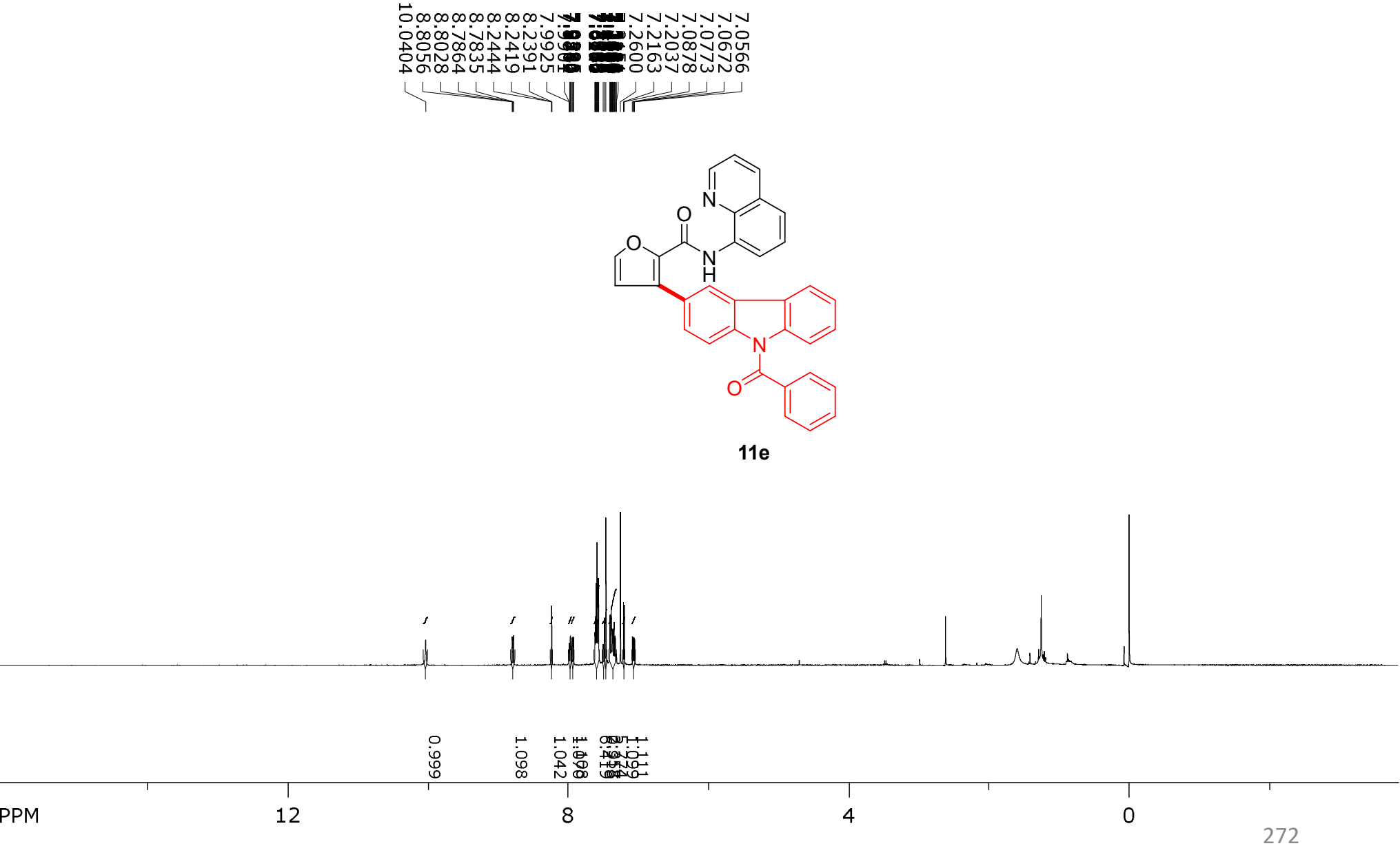
SpinWorks 4: RD 315
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 47



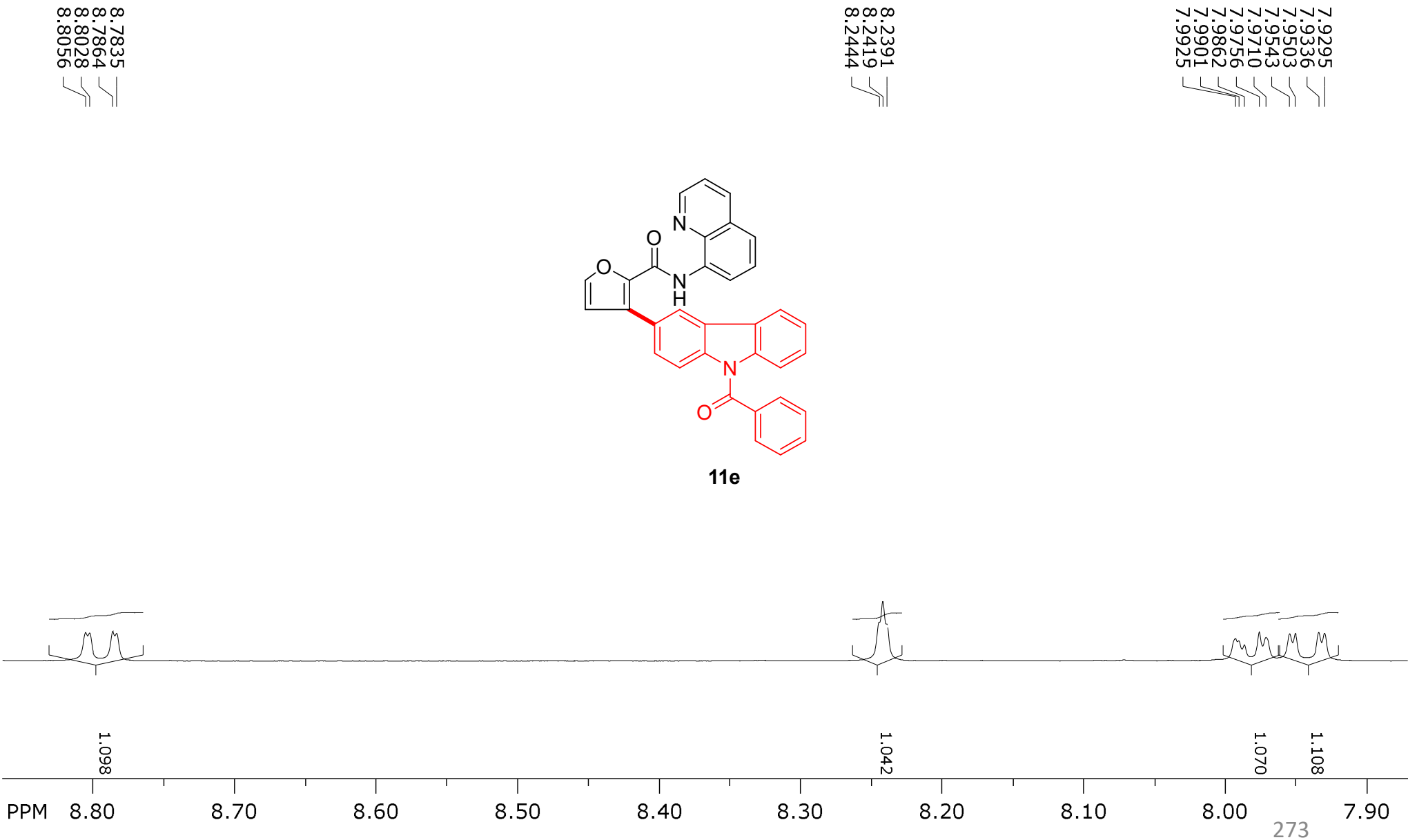
11d



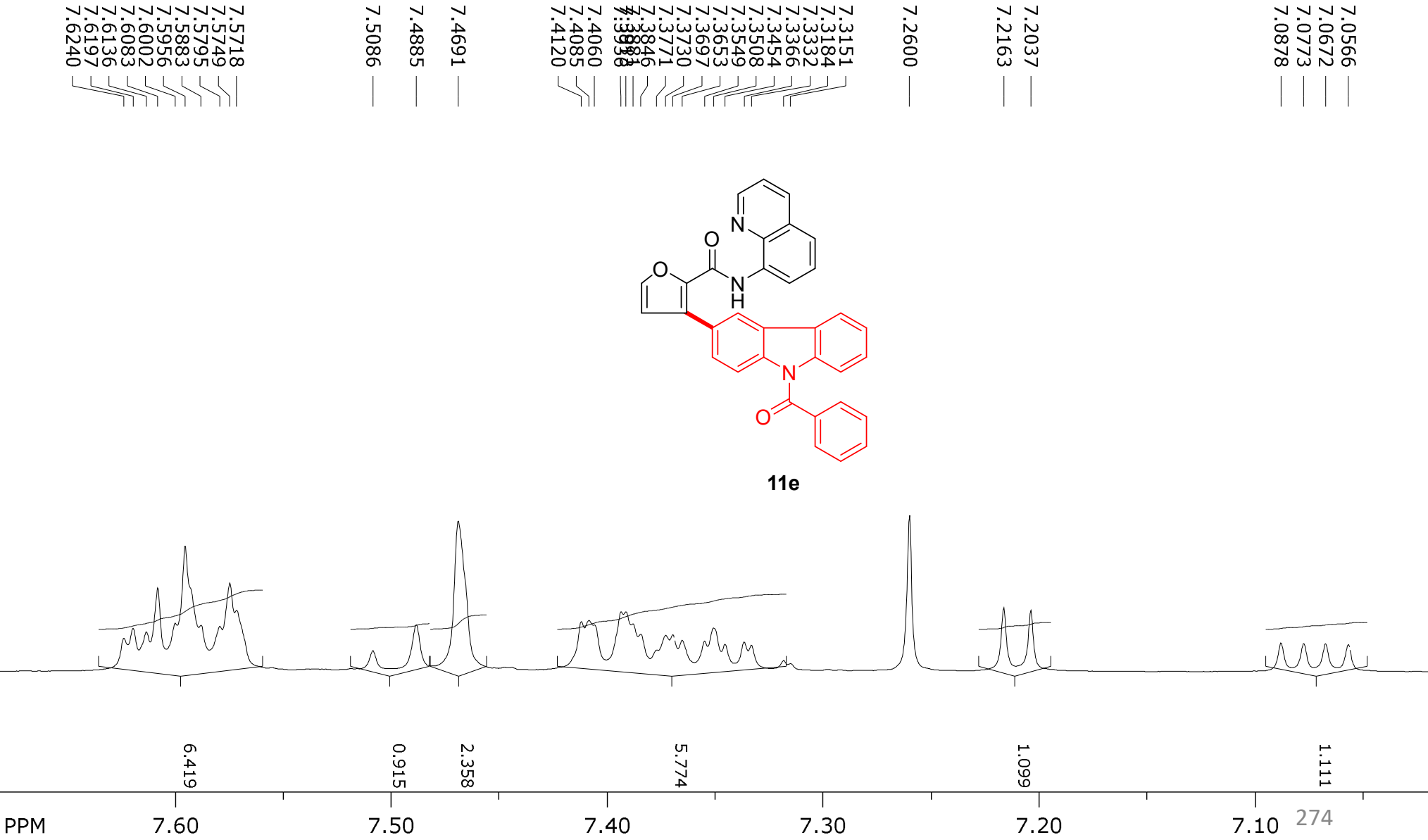
SpinWorks 4: rd-329-rep-1



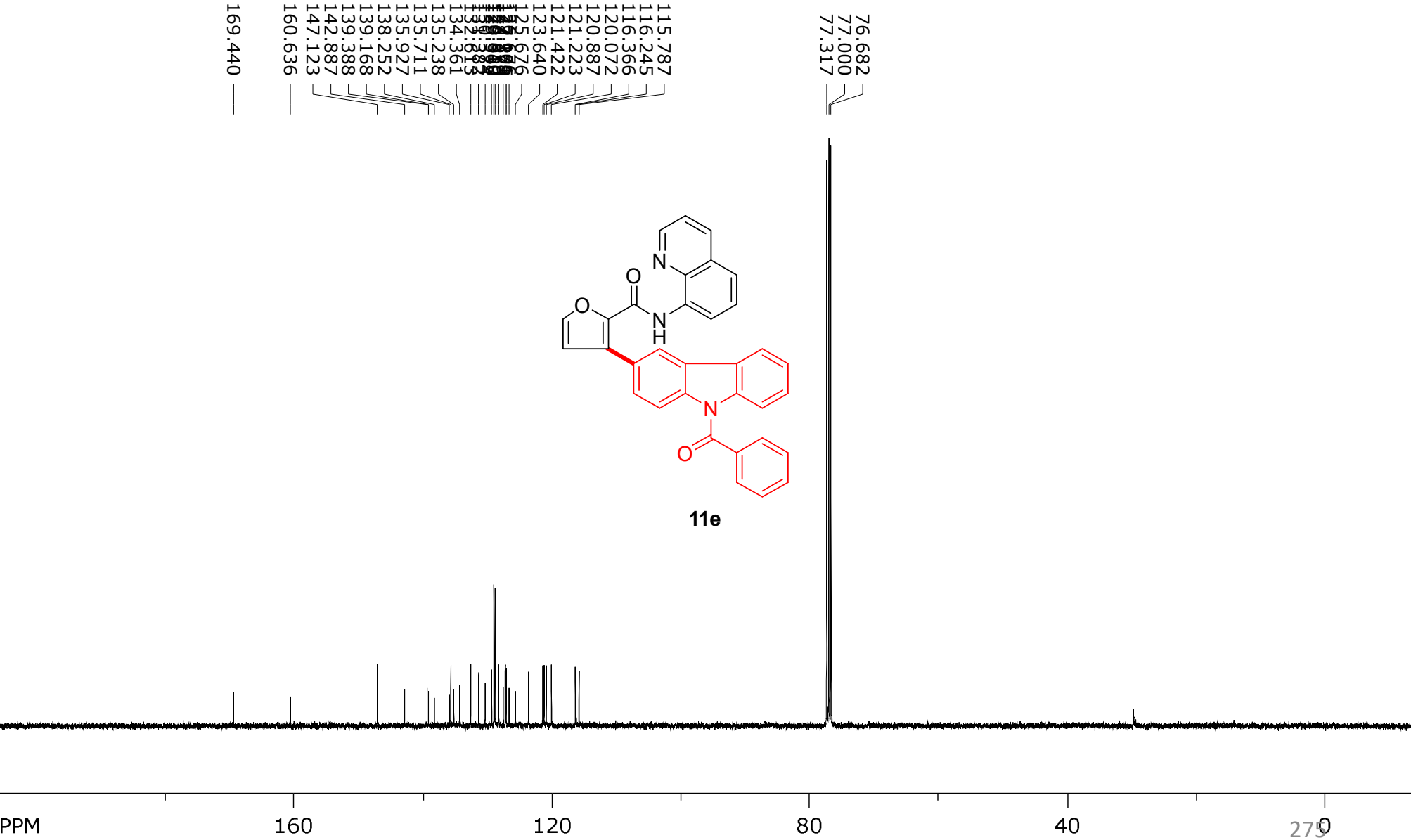
SpinWorks 4: rd-329-rep-1



SpinWorks 4: rd-329-rep-1



SpinWorks 4: RD-329
C13CPD CDCl3 {D:\data} nmr 1



SpinWorks 4: RD-329
C13CPD CDCl3 {D:\data} nmr 1

169.440 —

160.636 —

147.123 —

142.887 —

139.388 —

138.252 —

135.927 —

135.711 —

135.238 —

134.361 —

132.613 —

131.382 —

130.374 —

129.368 —

129.010 —

128.850 —

128.259 —

127.579 —

127.255 —

127.101 —

126.676 —

125.640 —

121.422 —

121.223 —

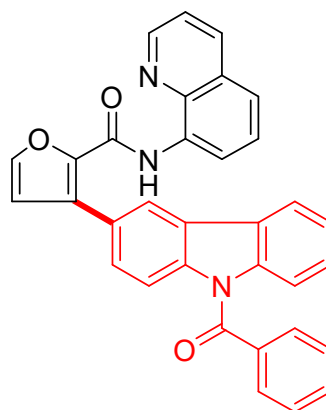
120.887 —

120.072 —

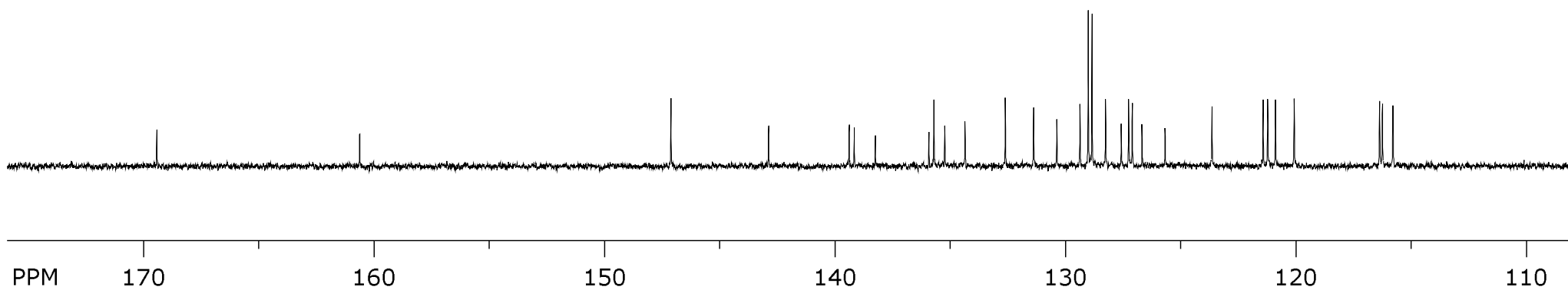
116.366 —

116.245 —

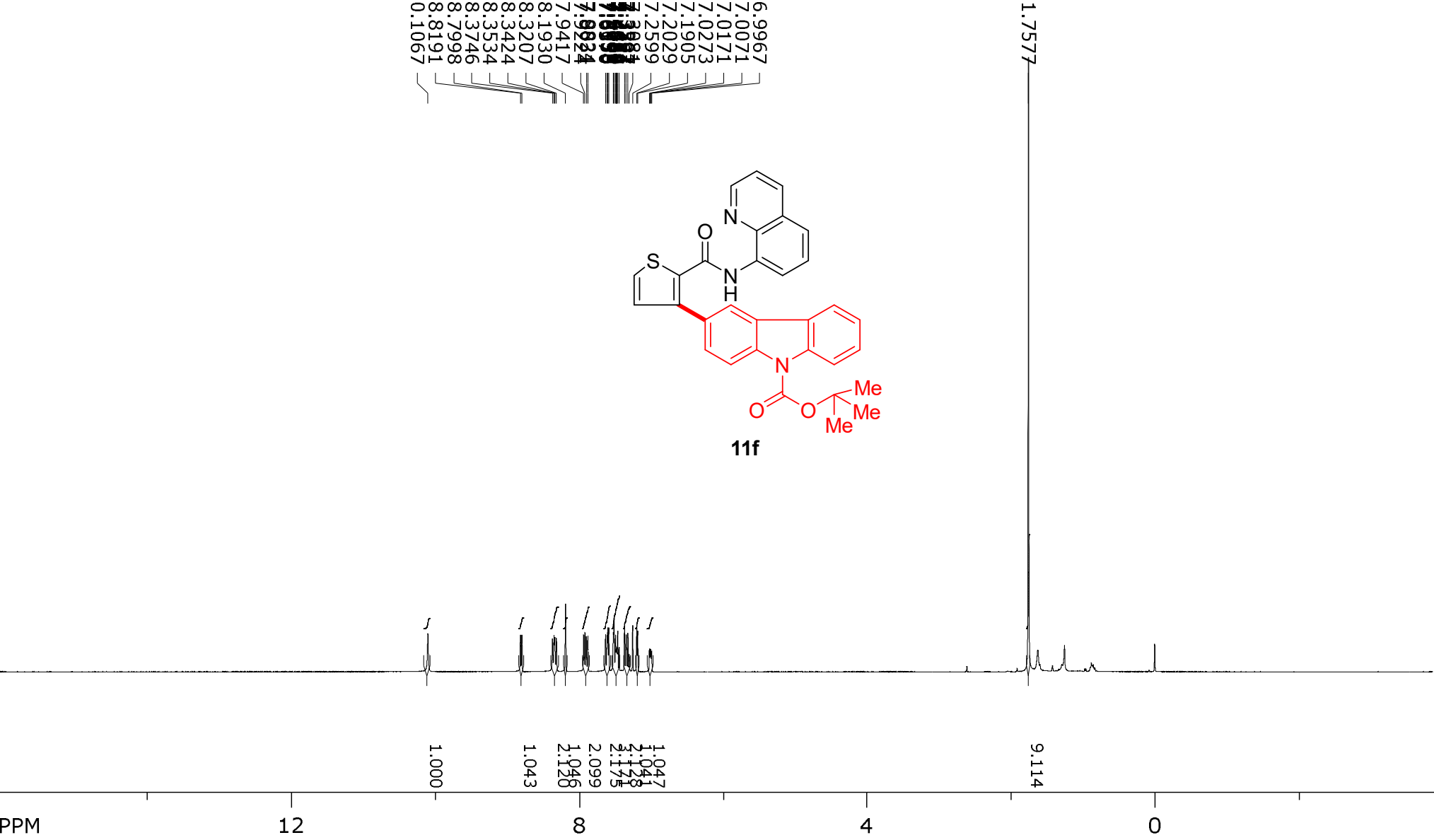
115.787 —



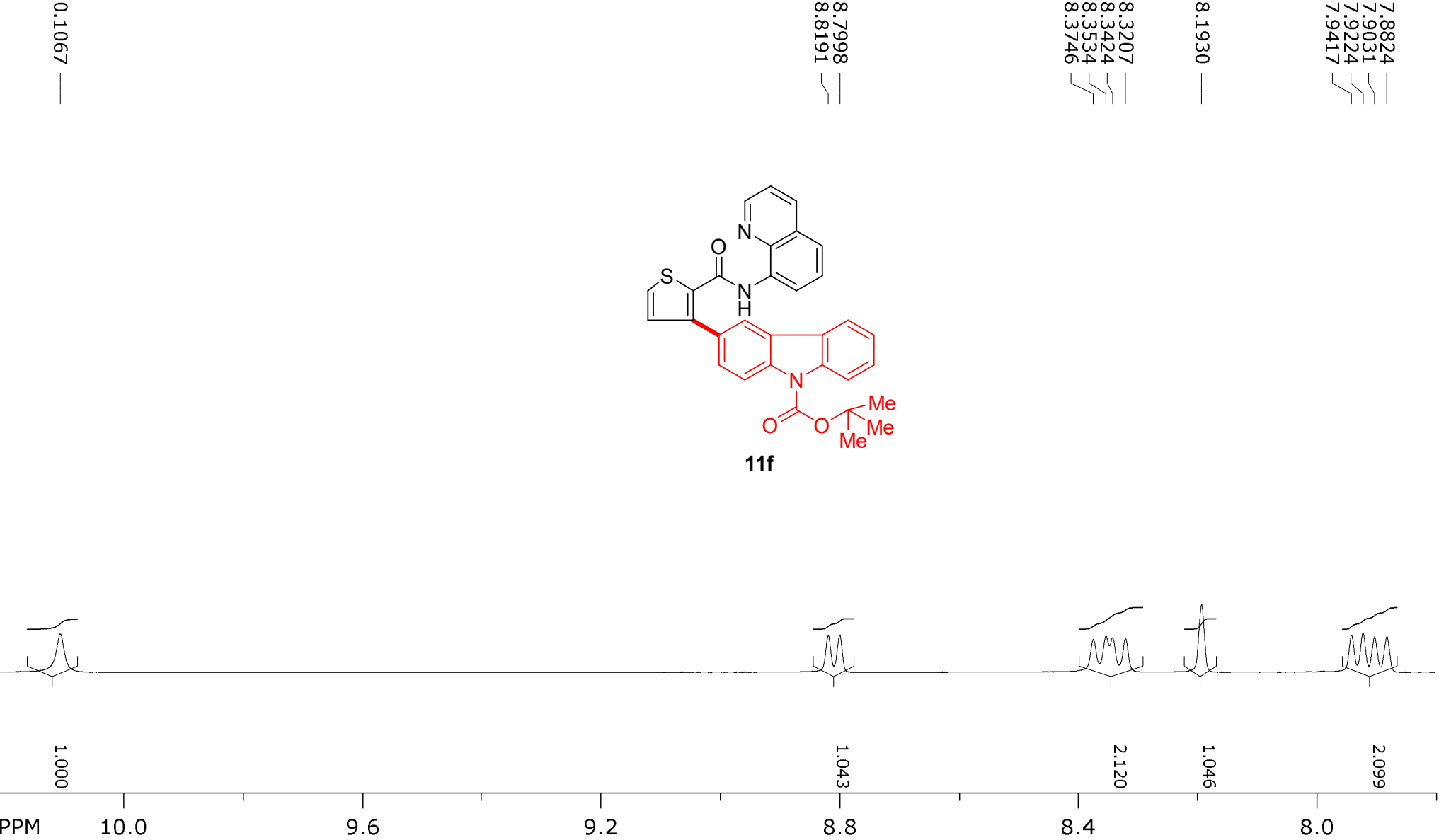
11e



SpinWorks 4: RD 319
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

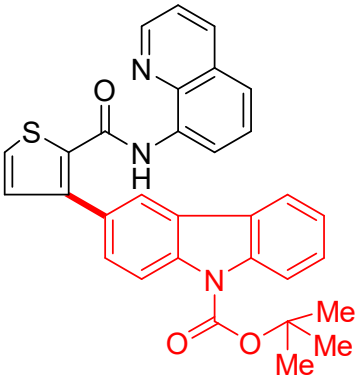


SpinWorks 4: RD 319
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

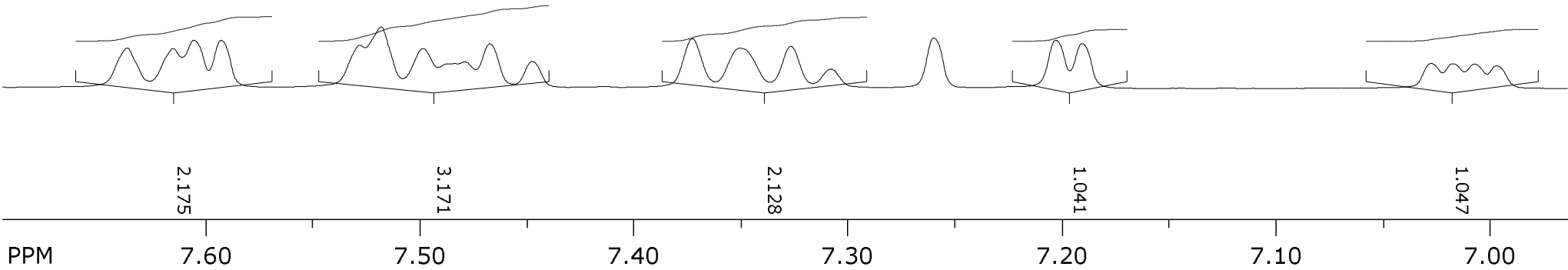


SpinWorks 4: RD 319
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

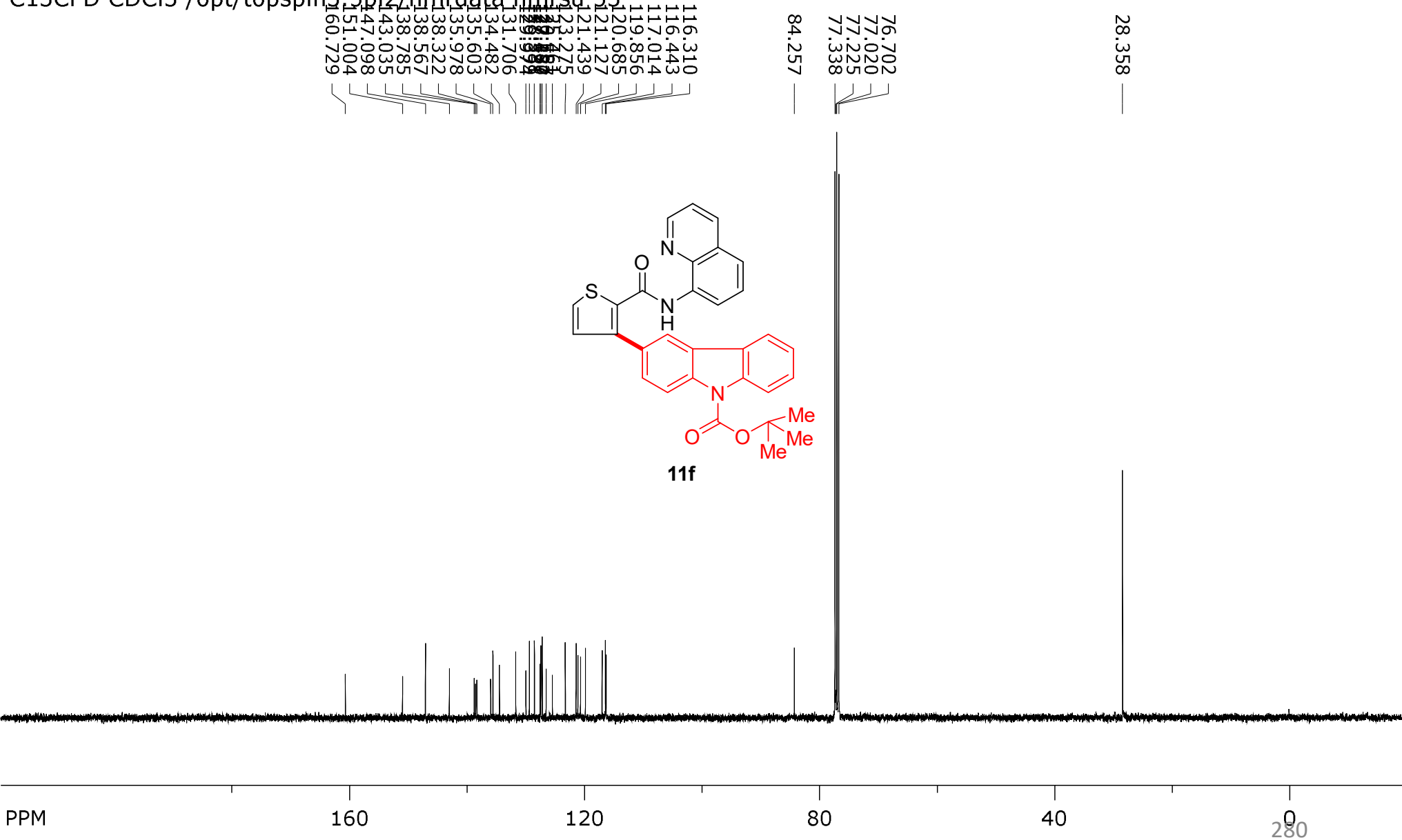
7.6370	7.5282	7.3727	7.2599	7.1905	7.0273
7.6155	7.5182	7.3502		7.2029	7.0171
7.5930	7.4986	7.3267			7.0071
	7.4865	7.3081			6.9967
	7.4854				
	7.4837				
	7.4789				
	7.4674				
	7.4476				



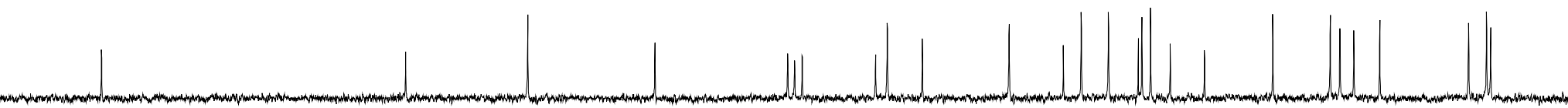
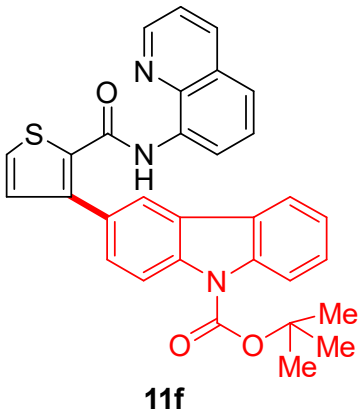
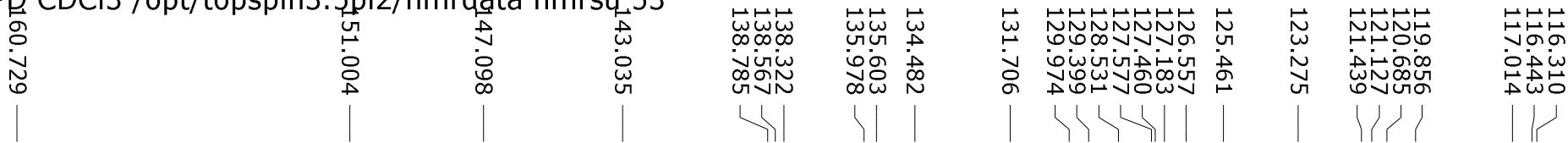
11f



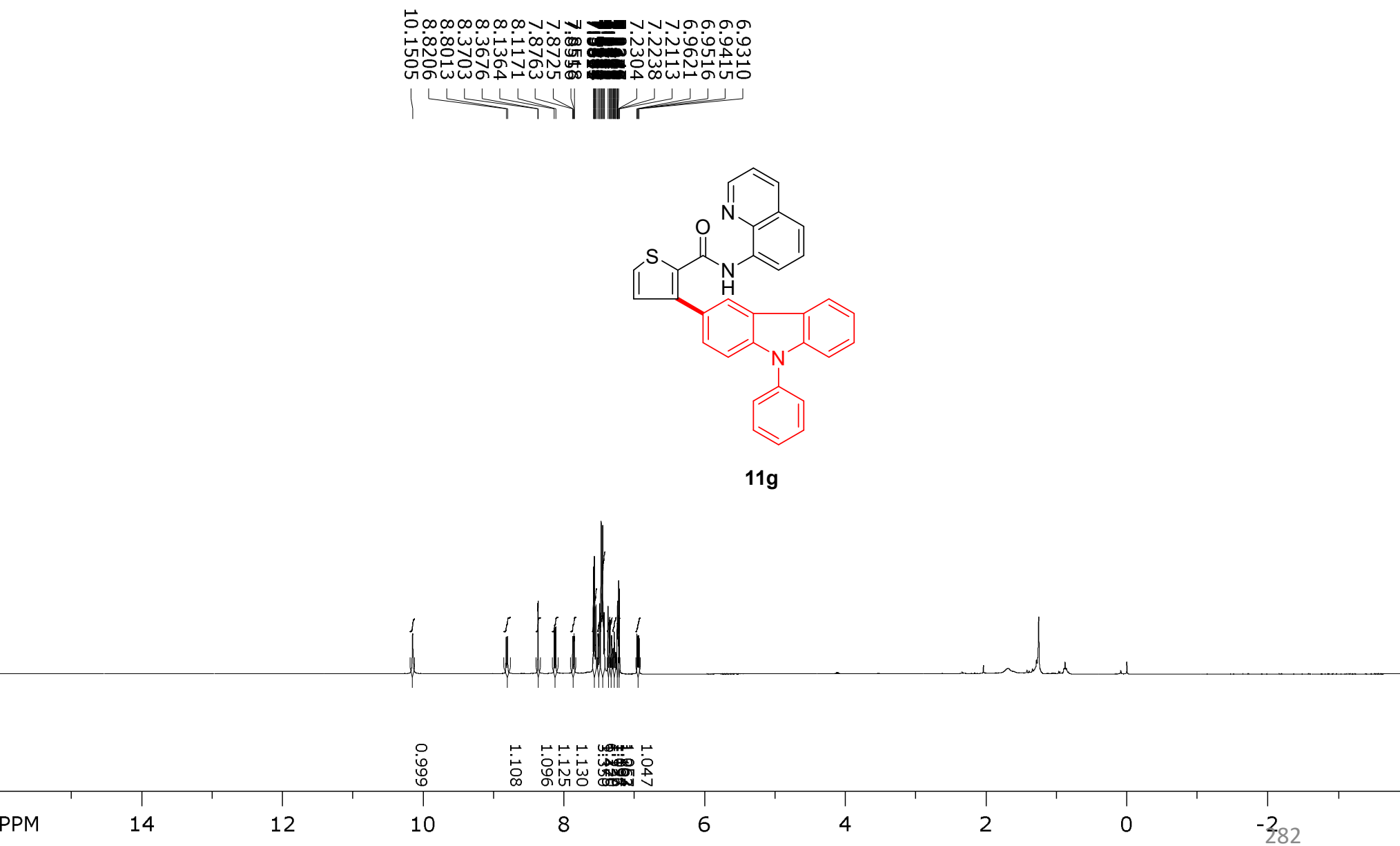
SpinWorks 4: RD 319
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53



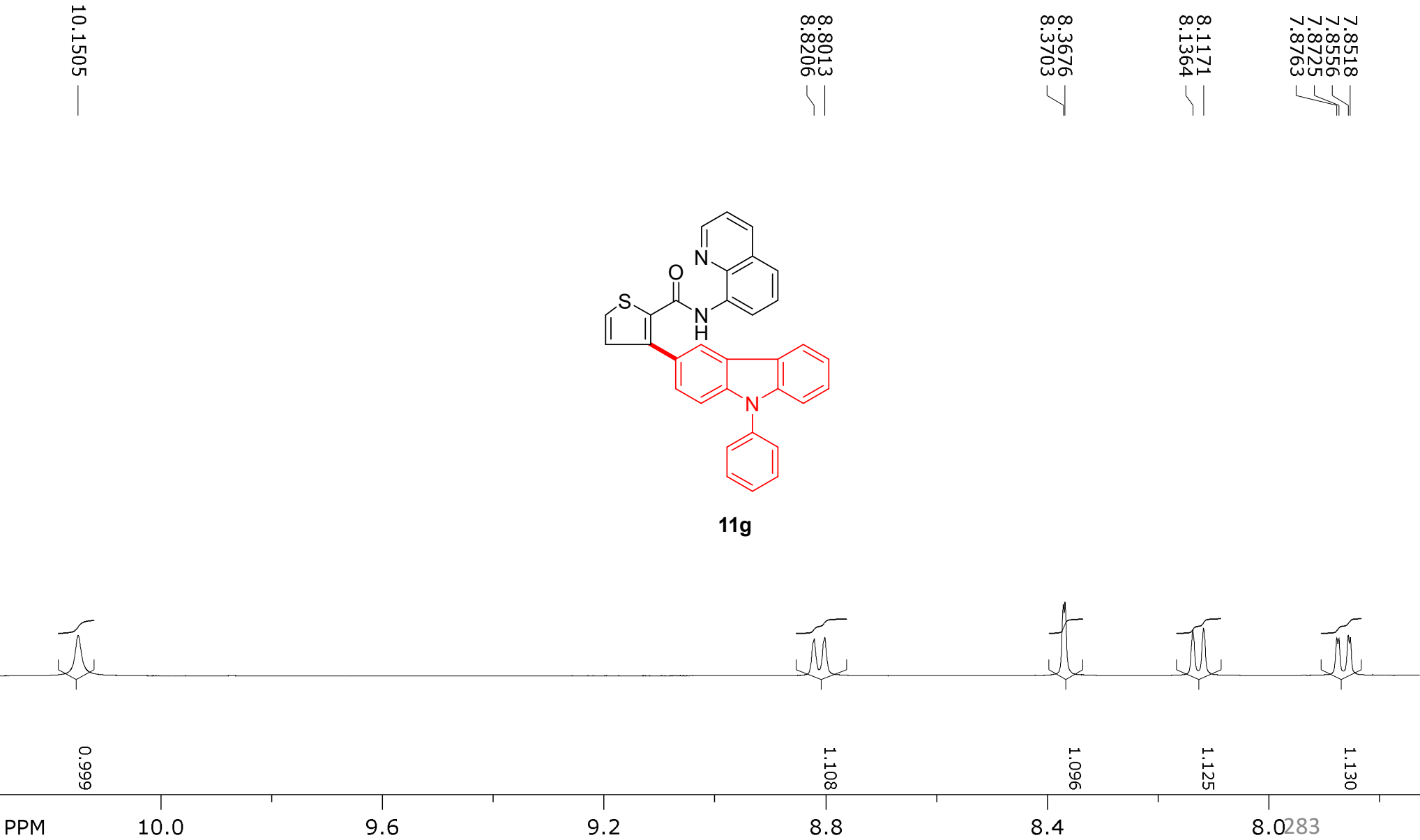
SpinWorks 4: RD 319
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

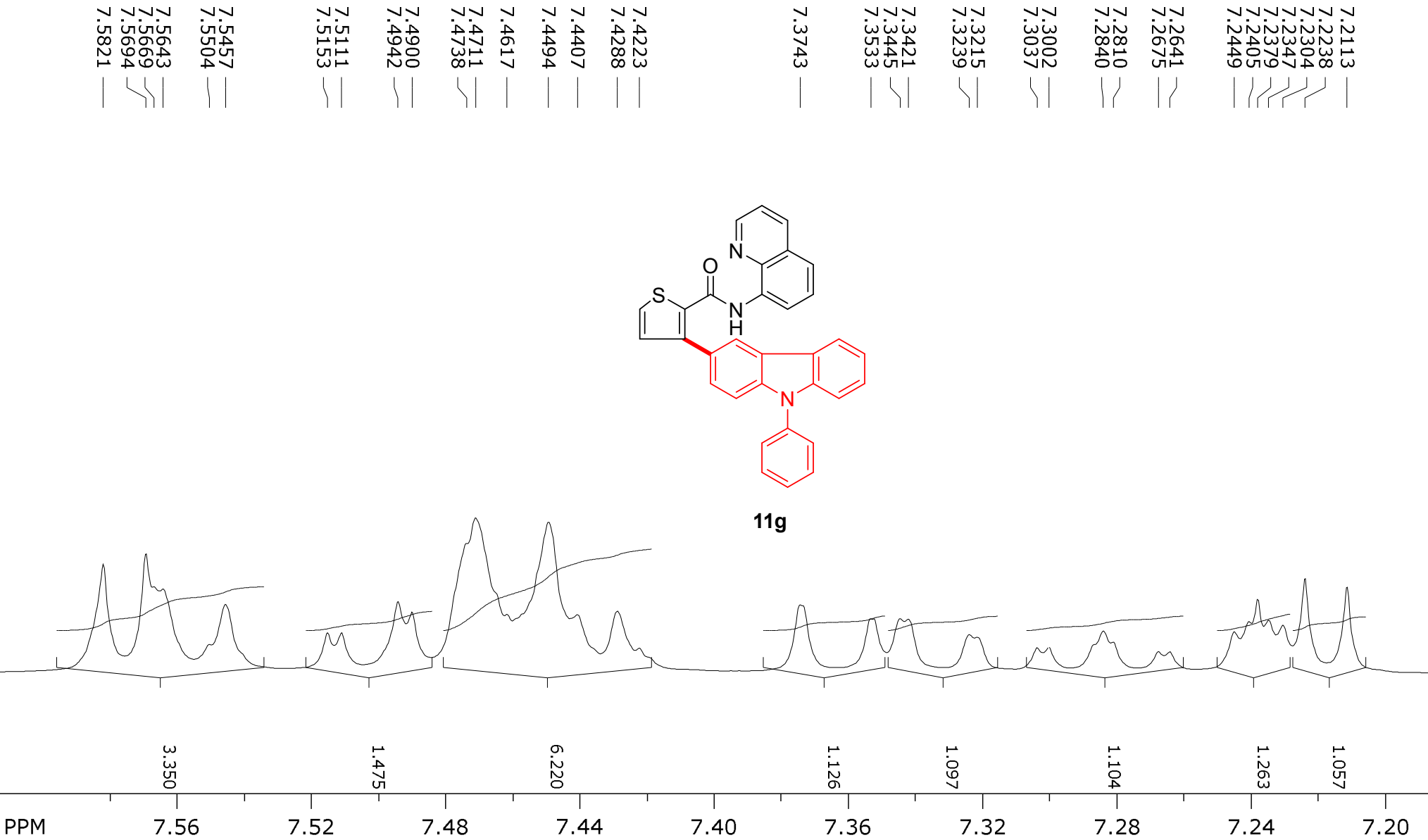


SpinWorks 4: Rd-285



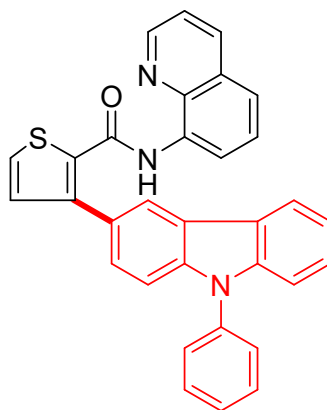
SpinWorks 4: Rd-285



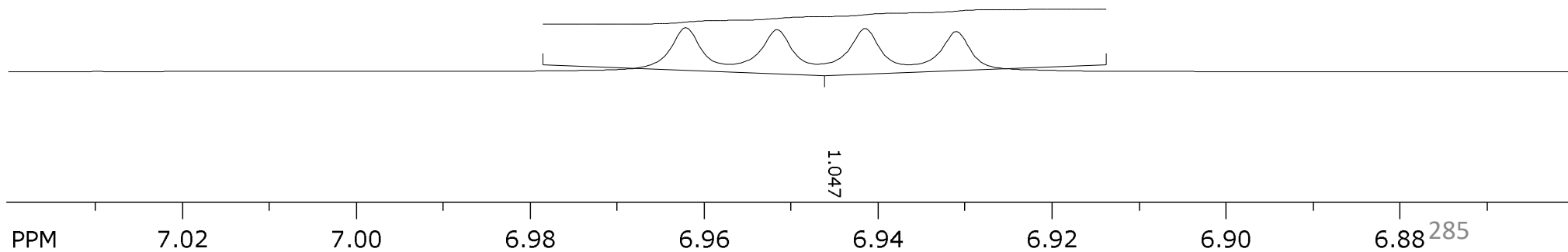


SpinWorks 4: Rd-285

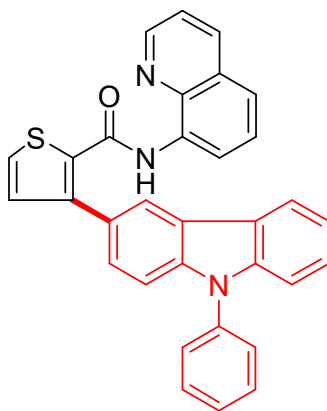
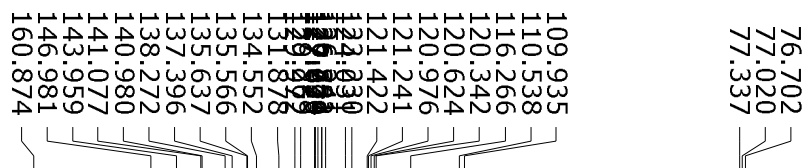
6.9310 —
6.9415 —
6.9516 —
6.9621 —



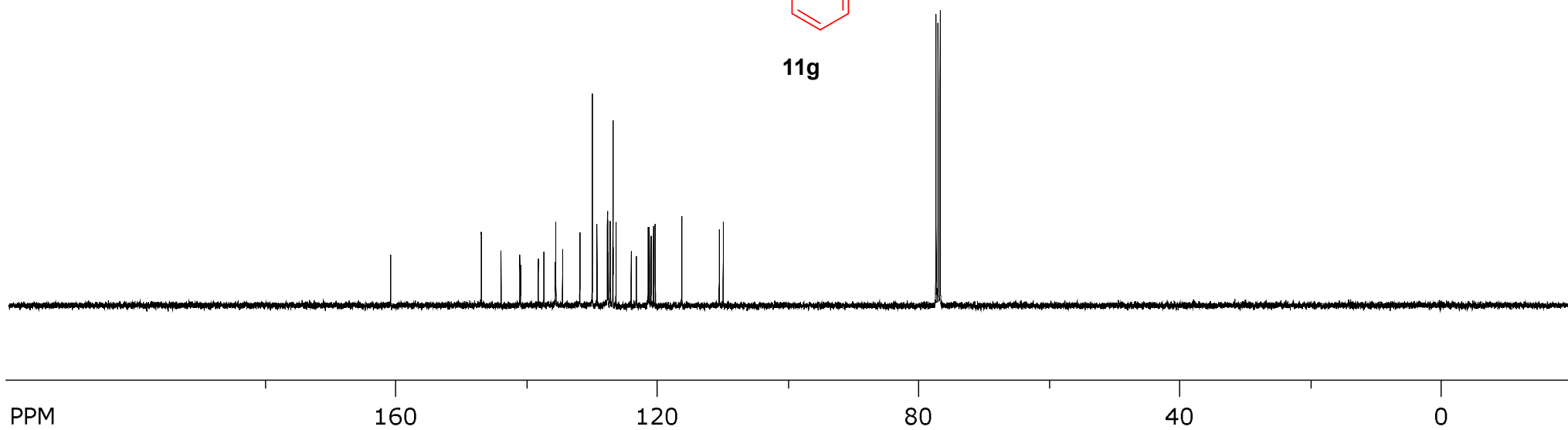
11g



13C

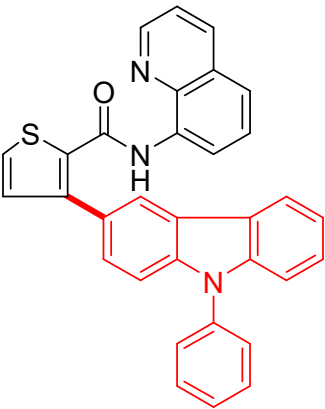
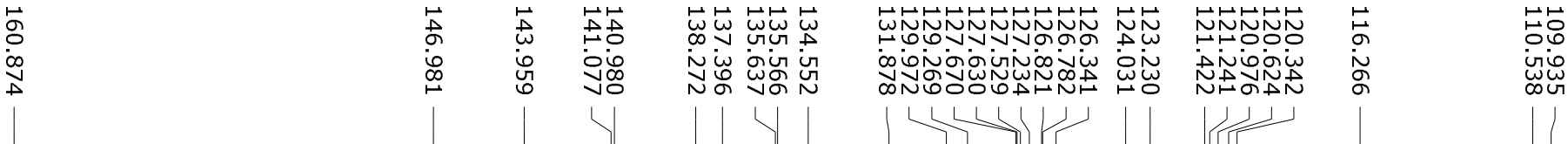


11g

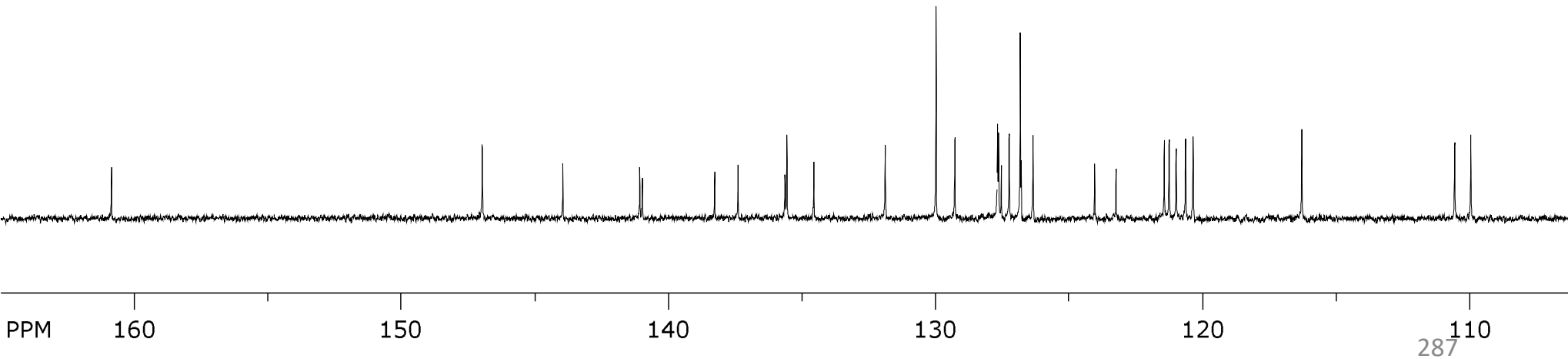


SpinWorks 4: rd 285

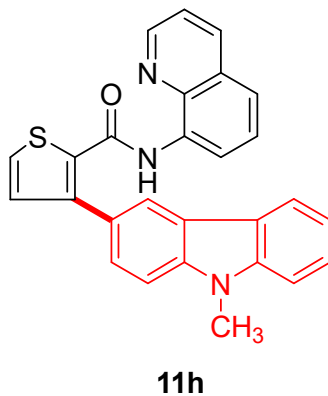
¹³C



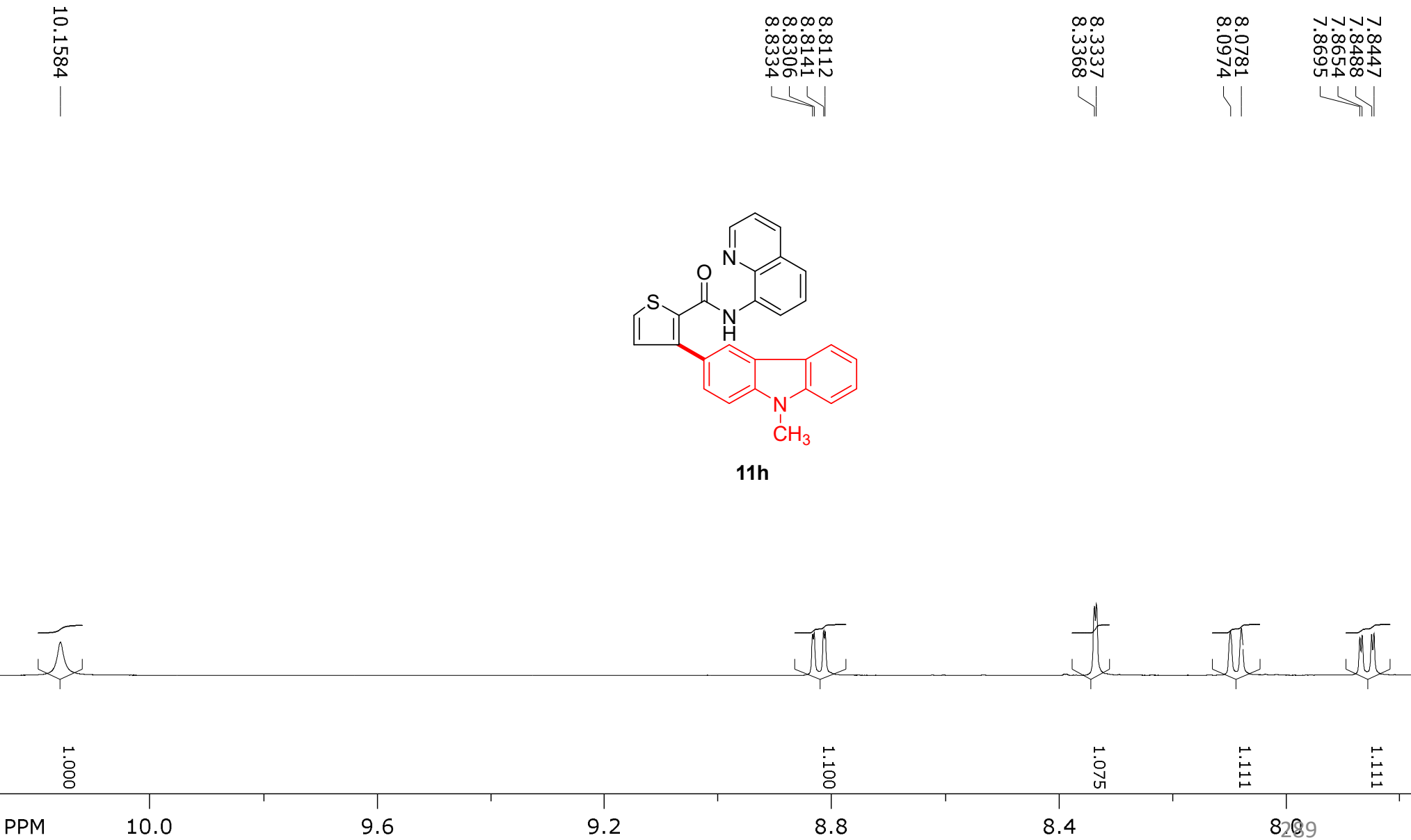
11g



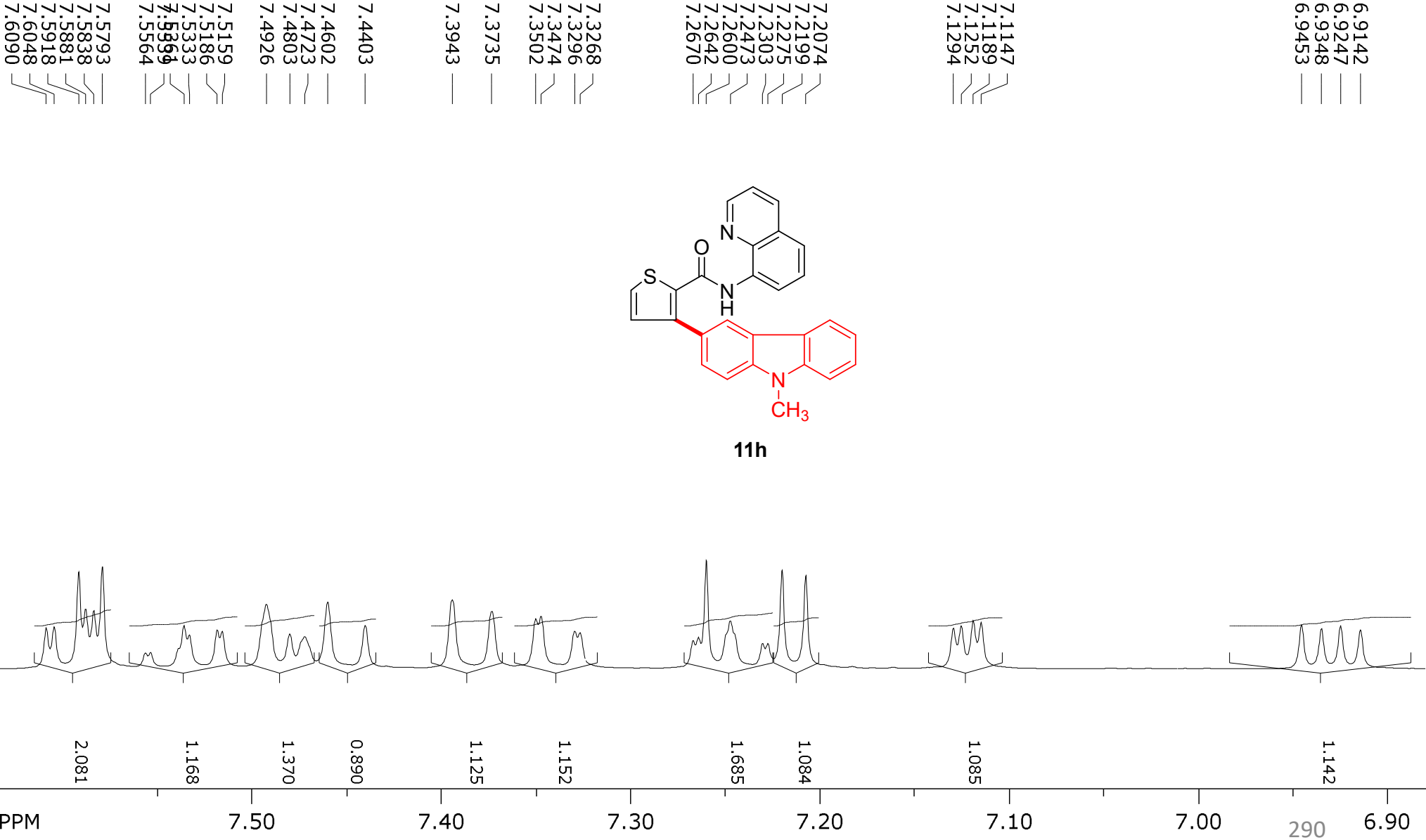
PPM



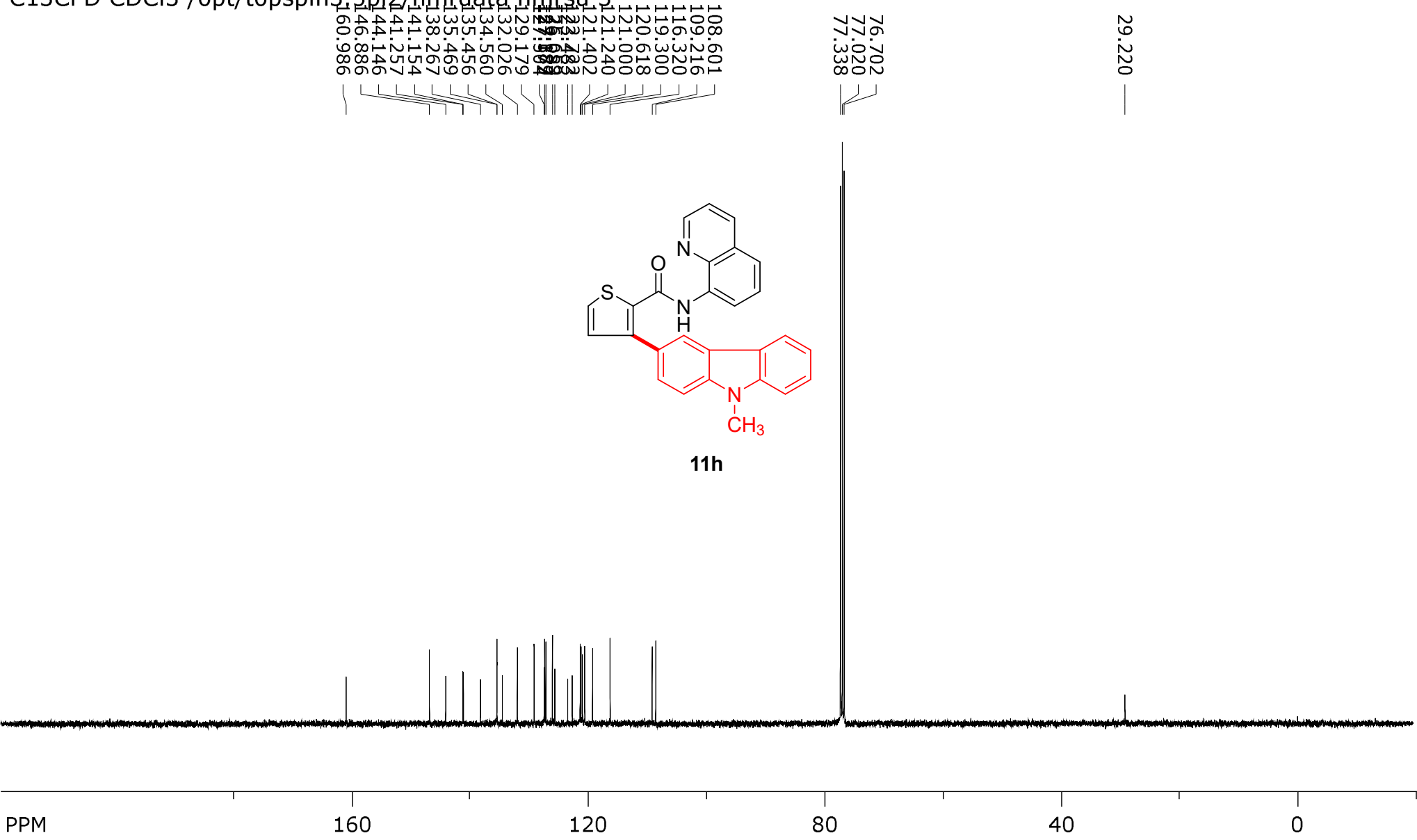
SpinWorks 4: rd-323



SpinWorks 4: rd-323

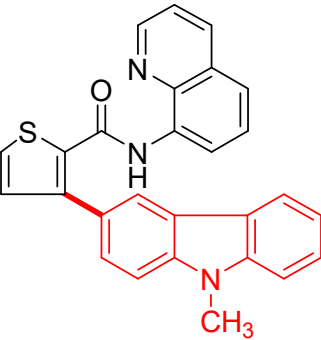


SpinWorks 4: RD 323
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

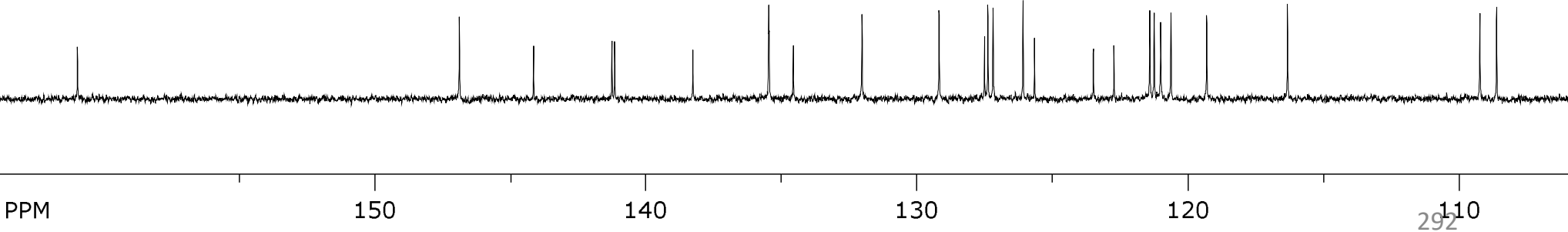


SpinWorks 4: RD 323
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

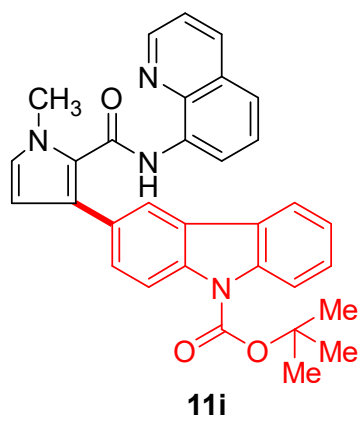
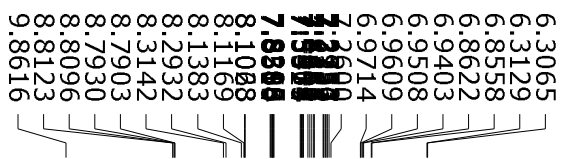
160.986 —
146.886 —
144.146 —
141.154 —
141.257 —
138.267 —
135.456 —
135.469 —
134.560 —
132.026 —
129.179 —
127.504 —
127.379 —
127.187 —
126.083 —
125.659 —
123.483 —
122.722 —
121.402 —
121.240 —
121.000 —
120.618 —
119.300 —
116.320 —
109.216 —
108.601 —



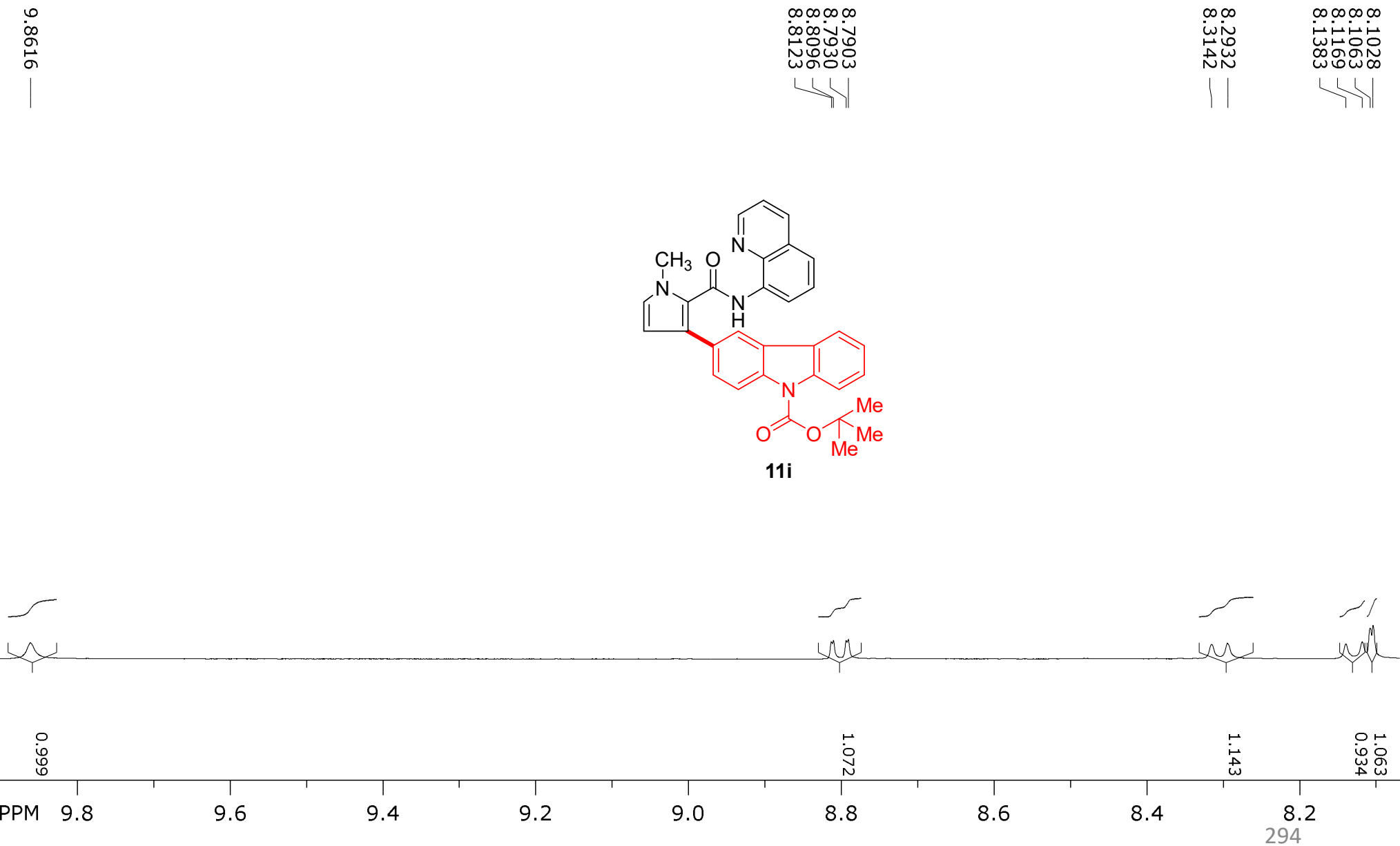
11h



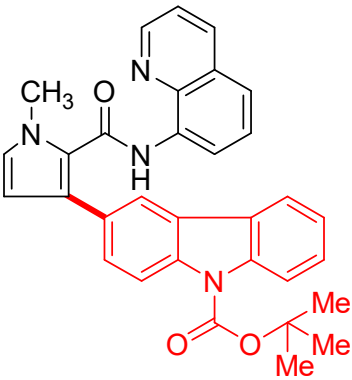
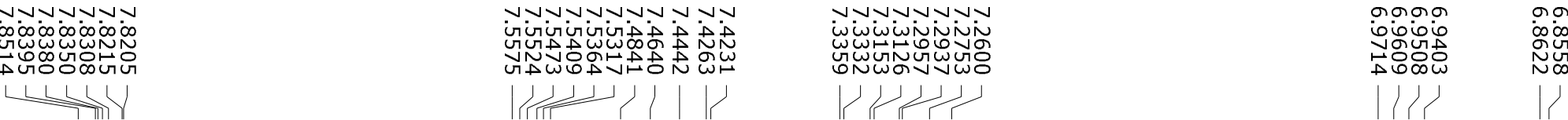
PPM



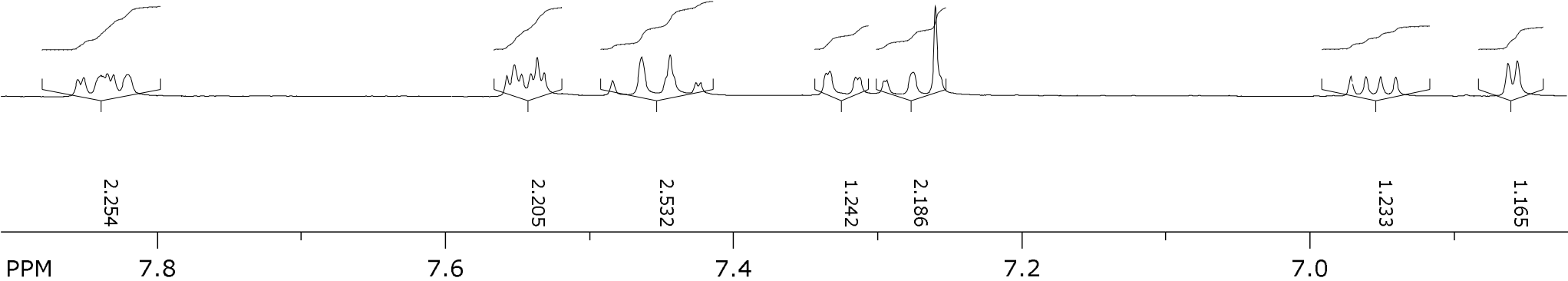
SpinWorks 4: rd-331



SpinWorks 4: rd-331



11i

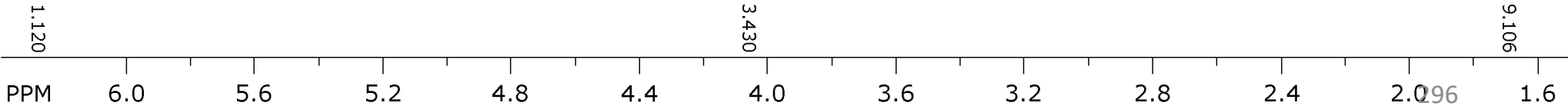
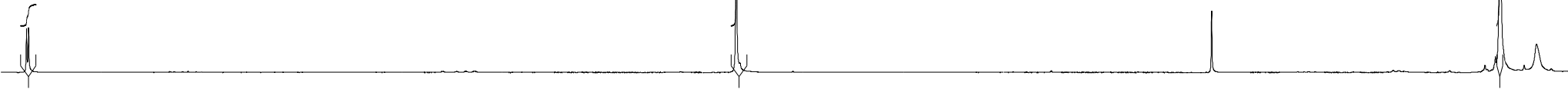
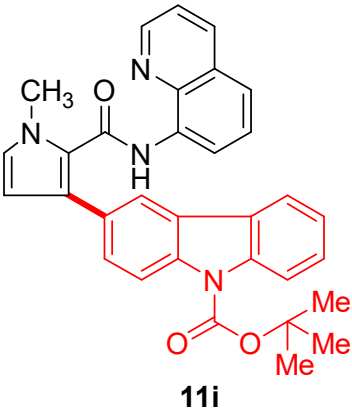


SpinWorks 4: rd-331

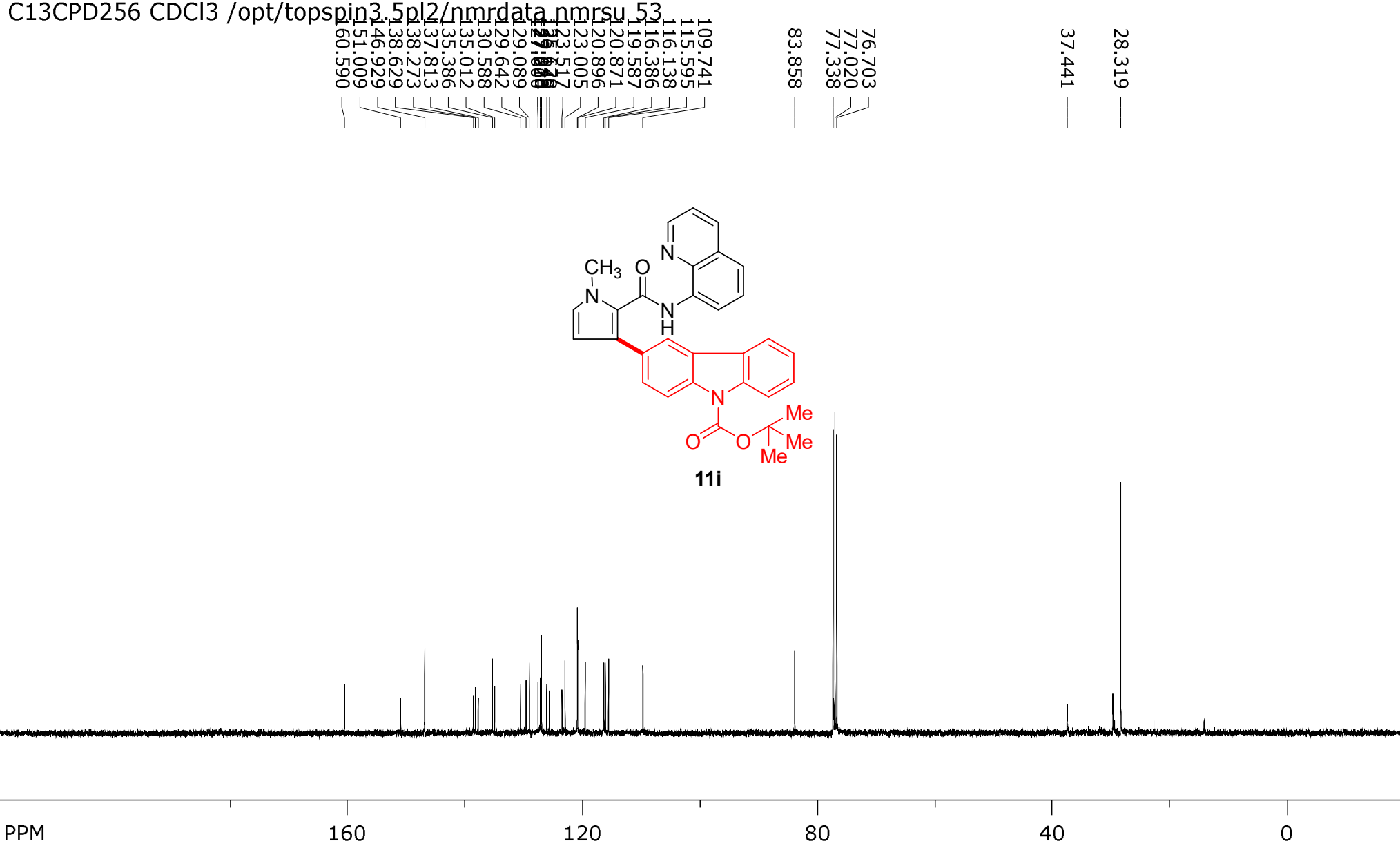
6.3065
6.3129

4.0987

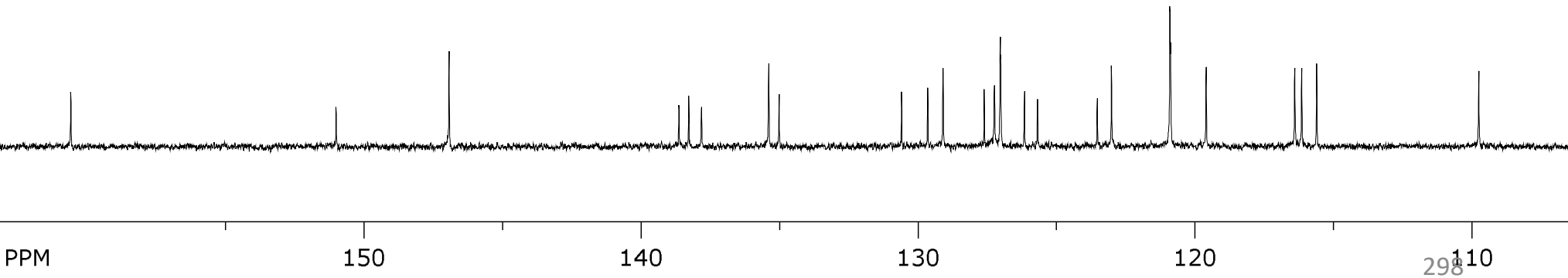
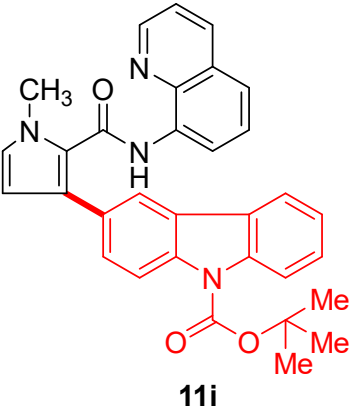
1.7155



SpinWorks 4: RD 331
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

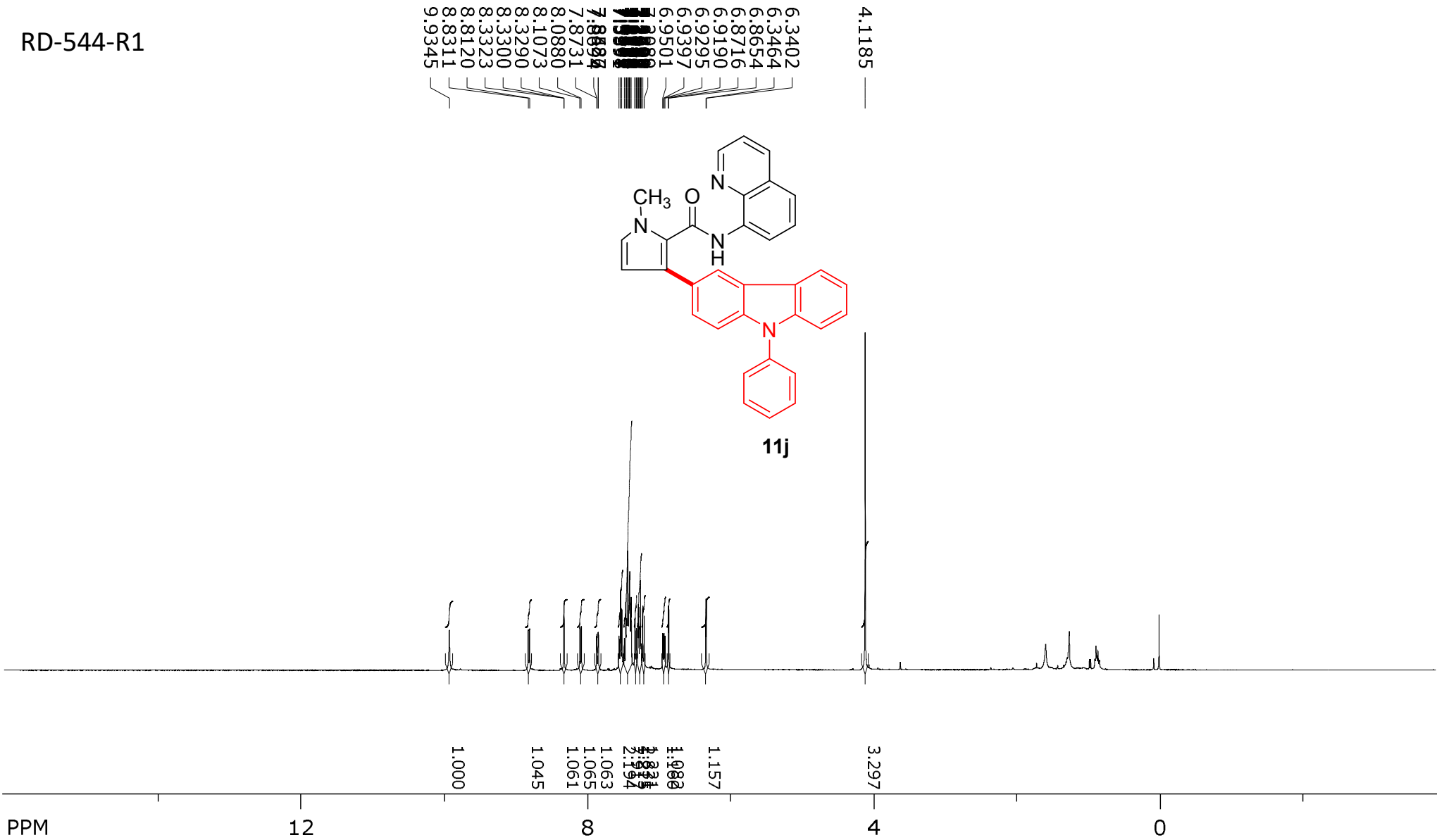


SpinWorks 4: RD 331
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53



SpinWorks 4: BENZ-T-NO2
1H

RD-544-R1



SpinWorks 4: BENZ-T-NO2
1H

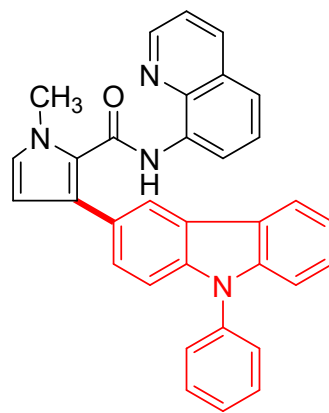
9.9345

8.8120
8.8311

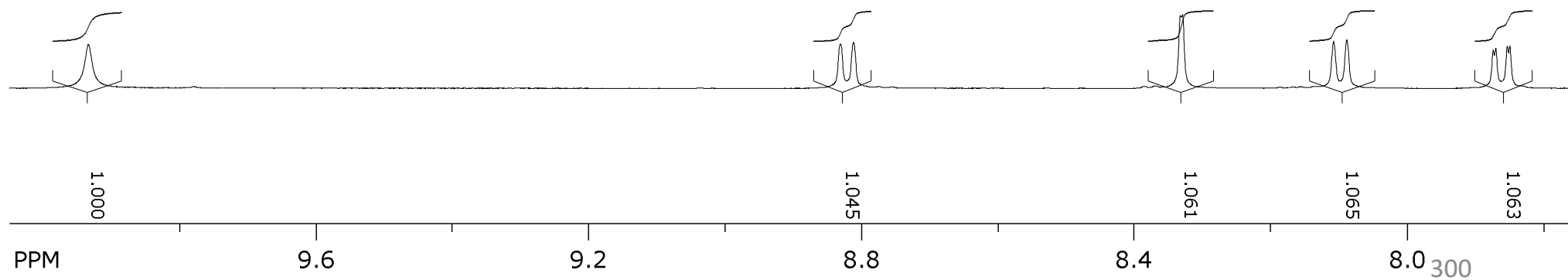
8.3290
8.3300
8.3323

8.0880
8.1073

7.8487
7.8526
7.8694
7.8731

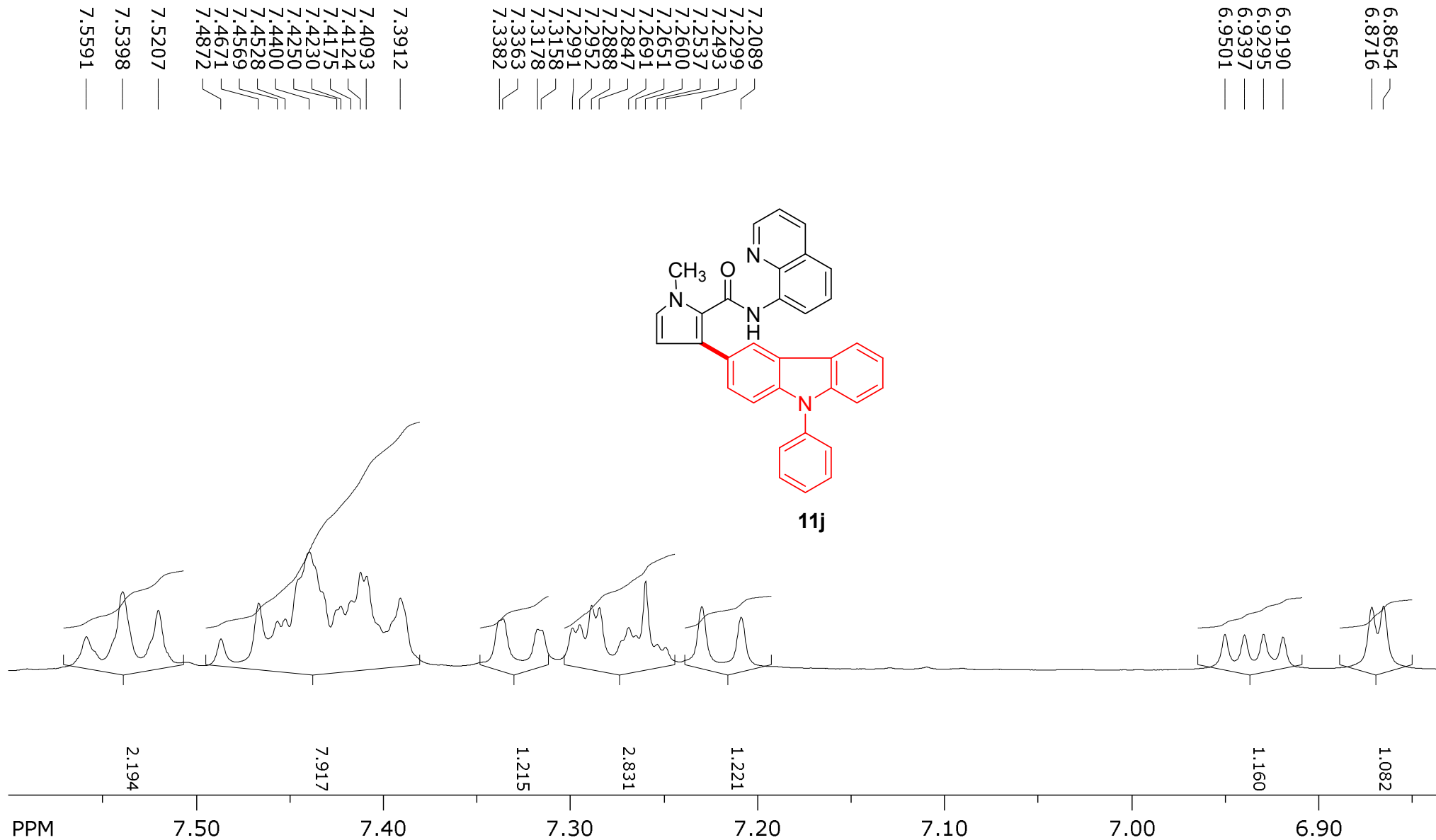


11j



SpinWorks 4: BENZ-T-NO2

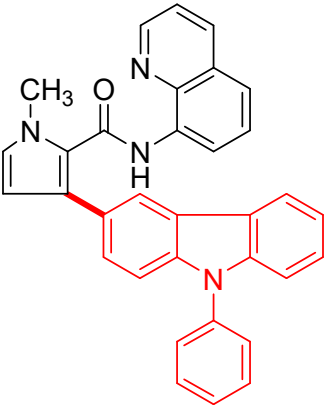
¹H



SpinWorks 4: BENZ-T-NO2
1H

6.3402
6.3464

4.1185



11j

1.157

3.297

302
4.0

PPM

6.4

6.0

5.6

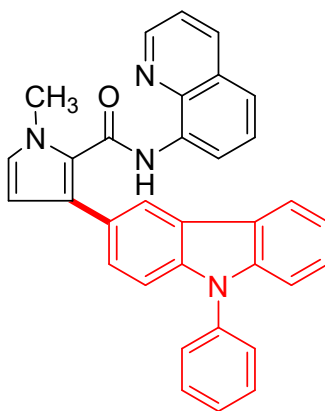
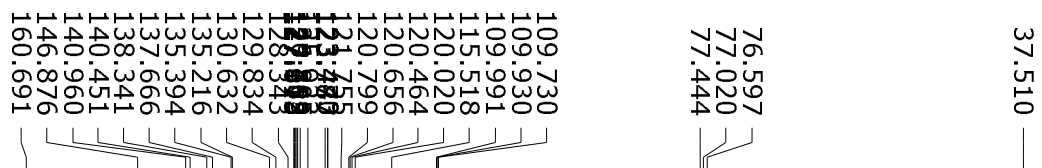
5.2

4.8

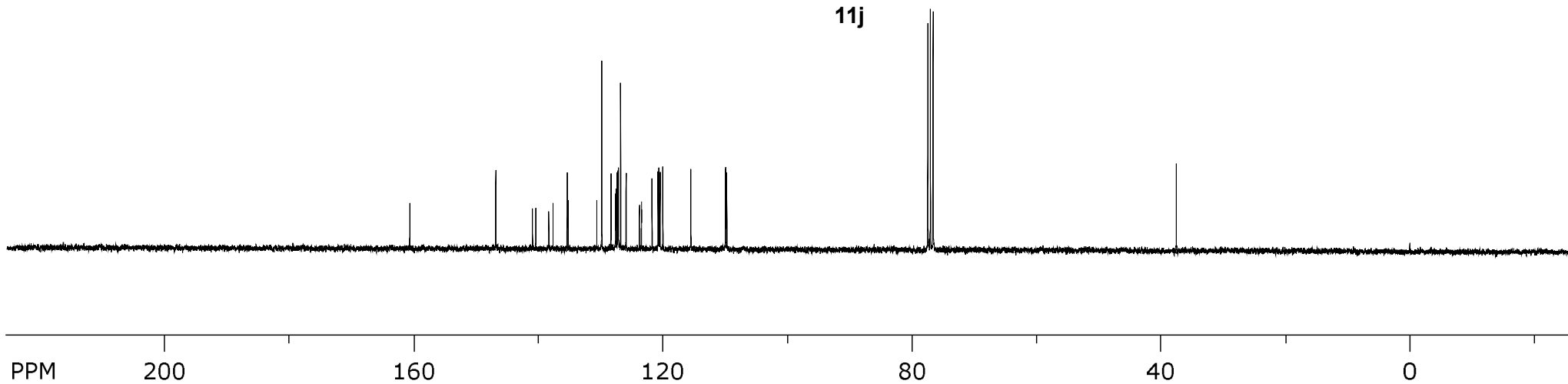
4.4

SpinWorks 4: SAB-73

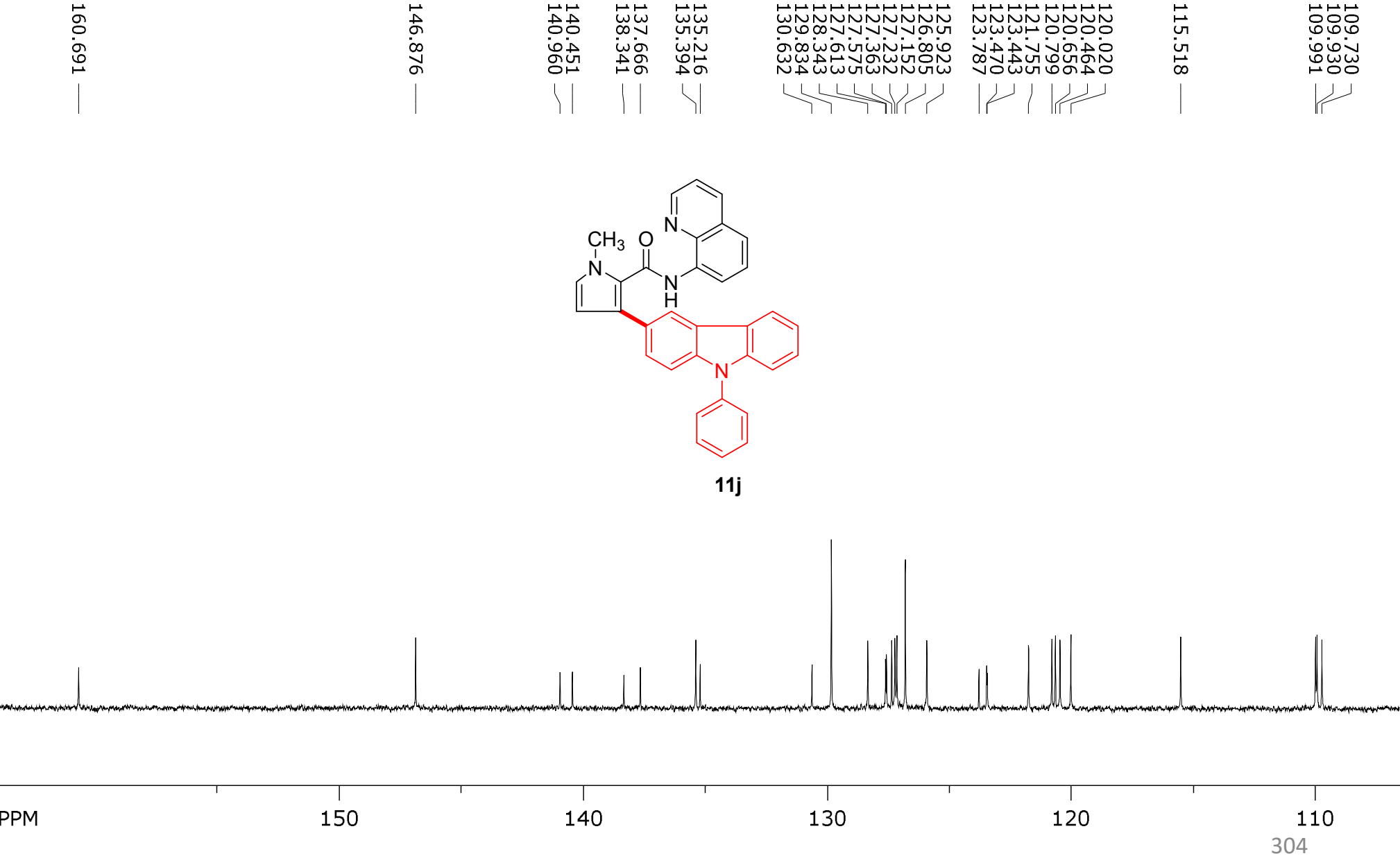
RD-544-R1



11j



SpinWorks 4: SAB-73



1H



SpinWorks 4: RD 635

¹H

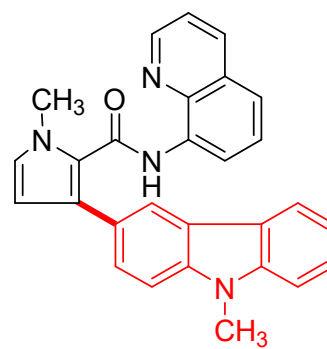
9.9160

8.8010
8.8203

8.2826

8.0371
8.0564

7.8168
7.8374



11k

0.999

1.035

1.047

1.076

1.063

PPM

9.6

9.2

8.8

8.4

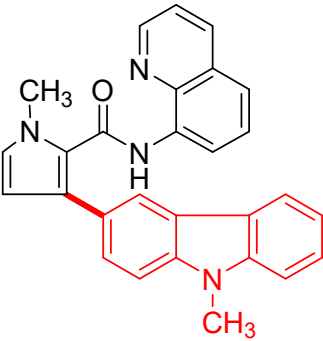
8.0

306

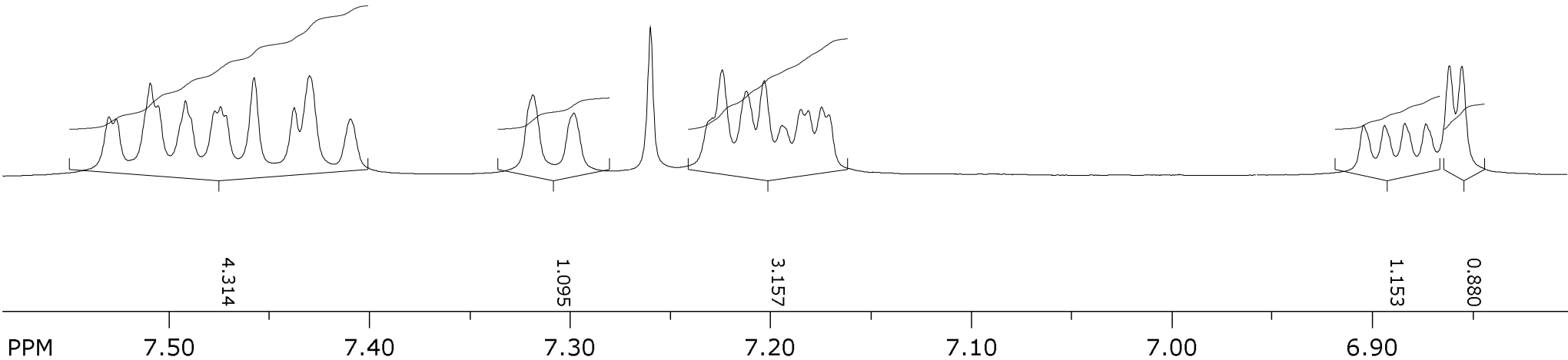
SpinWorks 4: RD 635

¹H

7.1709	7.1746	7.1813	7.1850	7.1943	7.2032	7.2121	7.2241	7.2289	7.2600	7.2982	7.3186	7.4098	7.4301	7.4378	7.4578	7.4720	7.4745	7.4773	7.4920	7.5058	7.5096	7.5265	7.5302
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
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11k

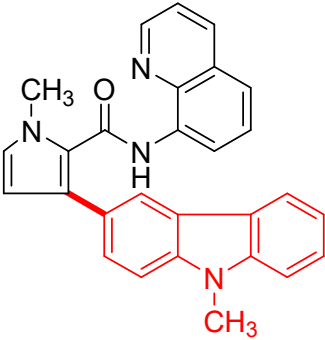


SpinWorks 4: RD 635
1H

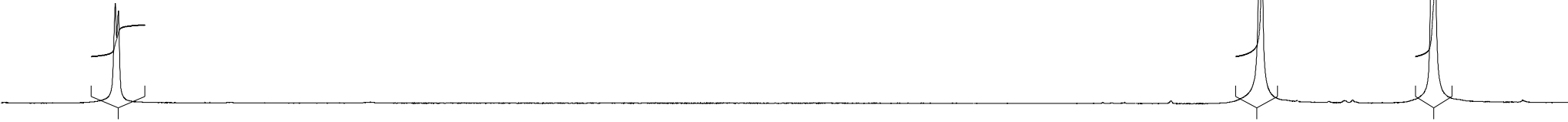
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6.3212

4.1105

3.7790



11k



1.096

3.147

3.173

PPM

6.0

5.6

5.2

4.8

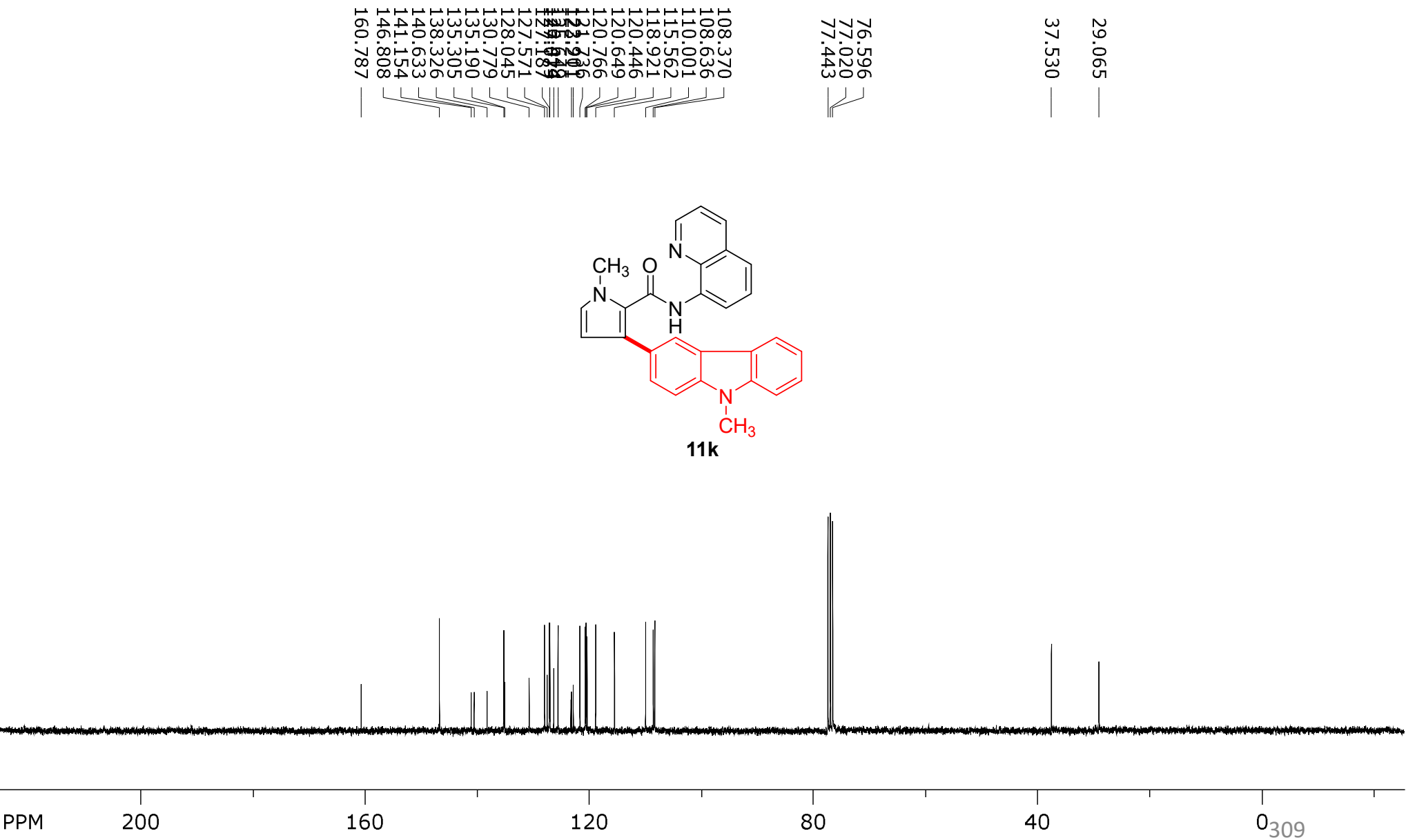
4.4

4.0

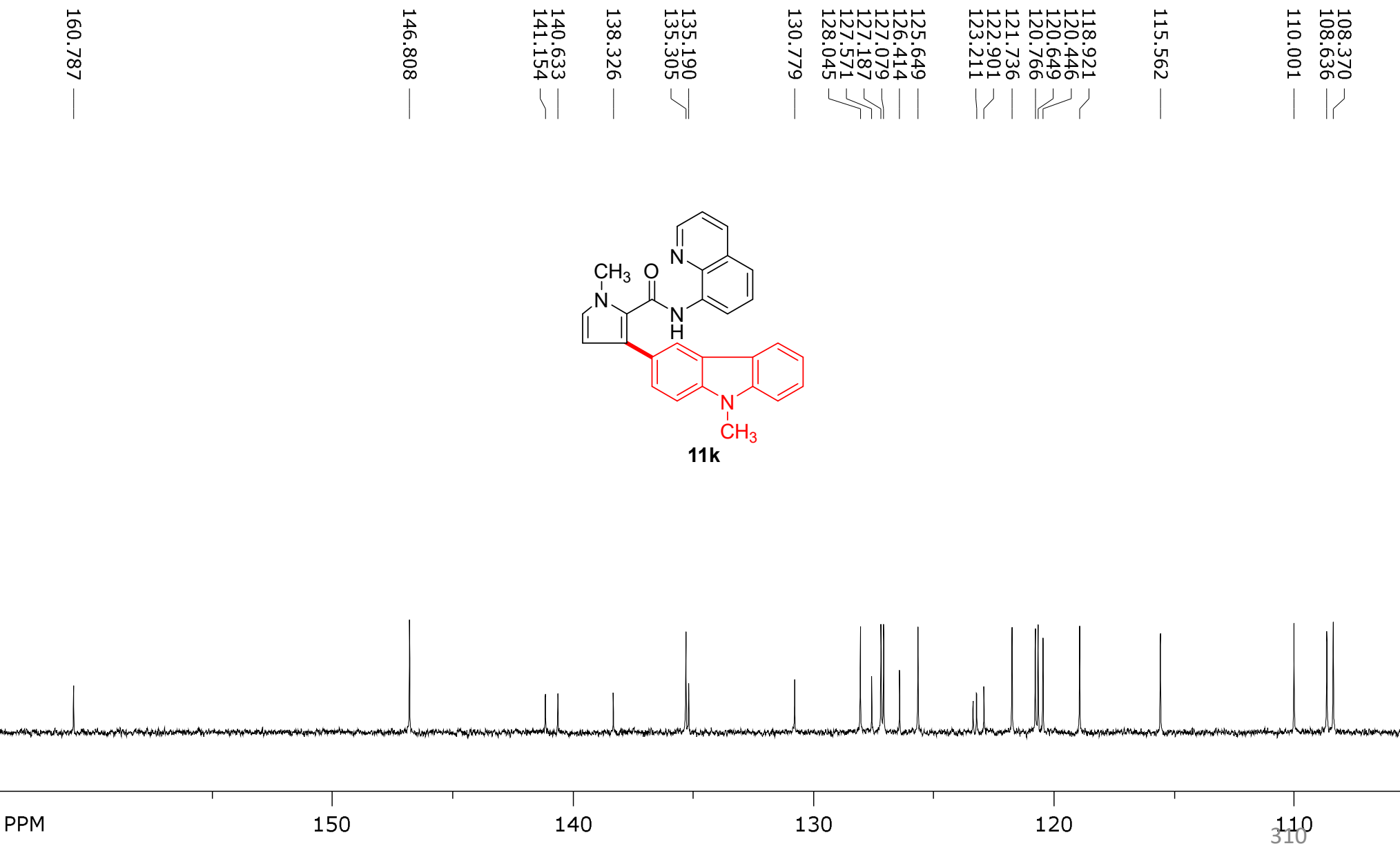
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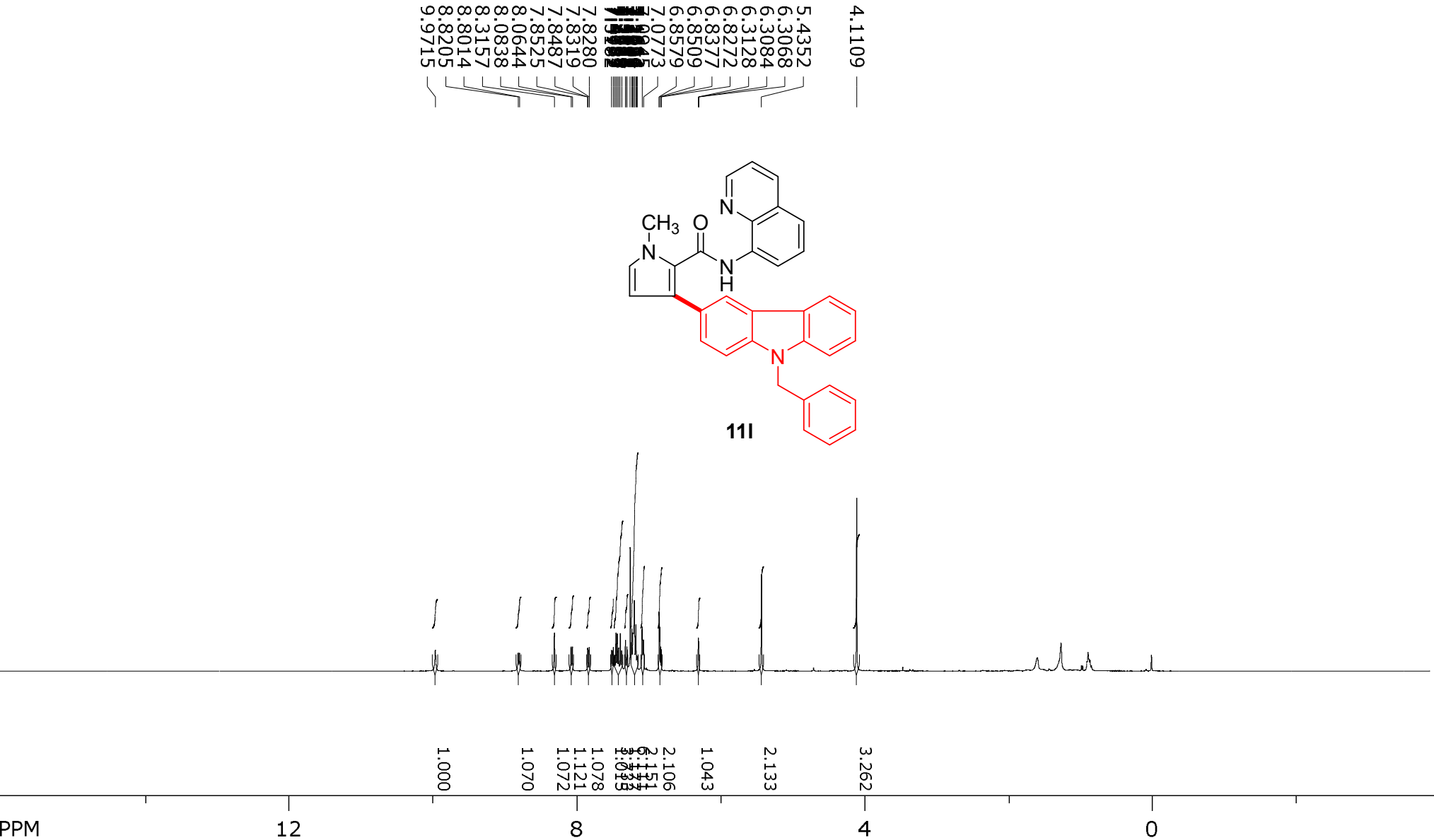
SpinWorks 4: SAB-85



SpinWorks 4: SAB-85

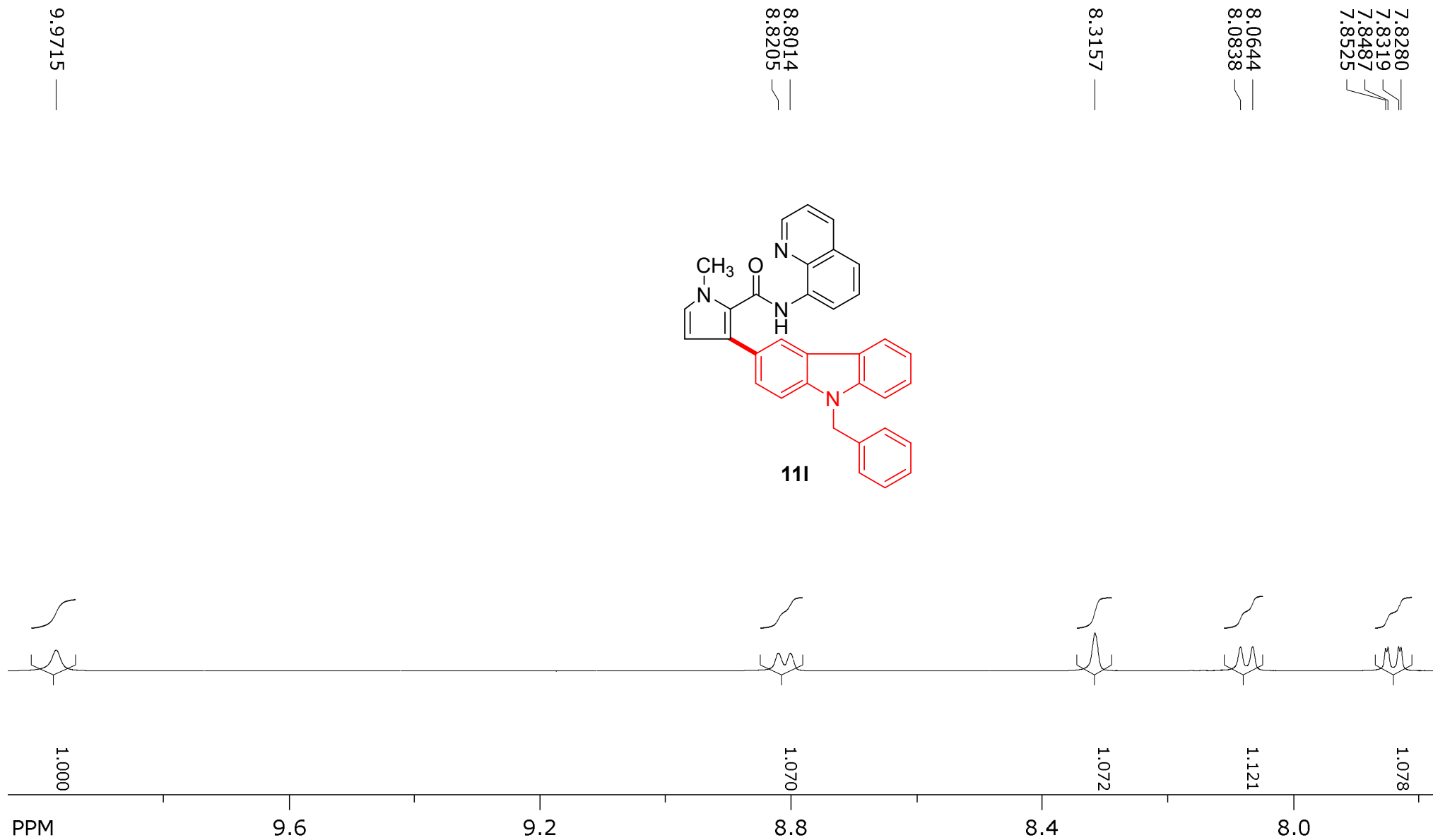


SpinWorks 4: RD 631
1H



SpinWorks 4: RD 631

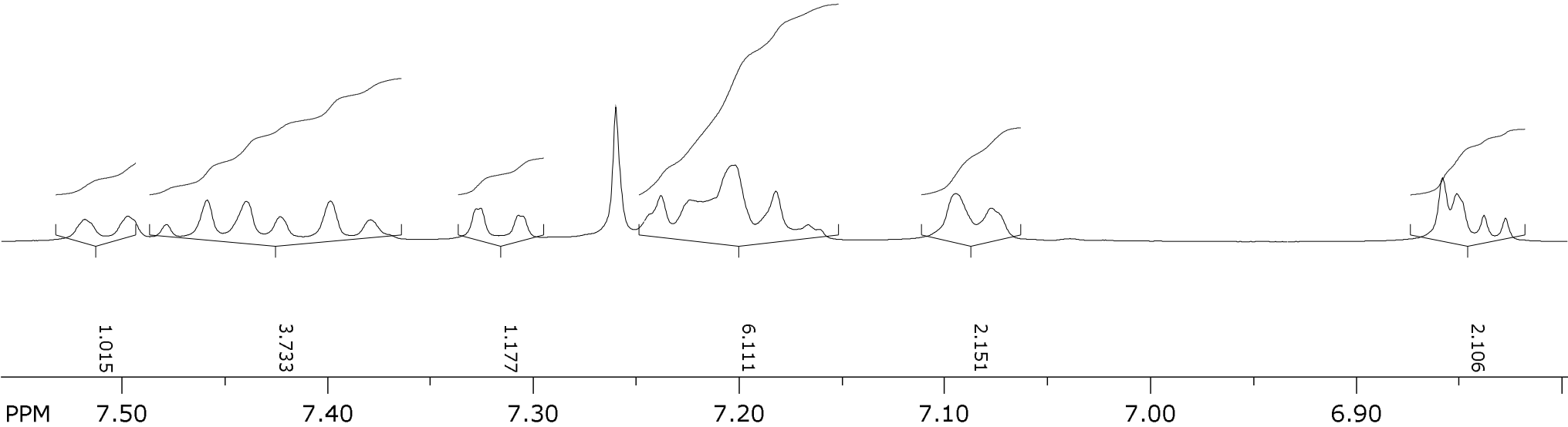
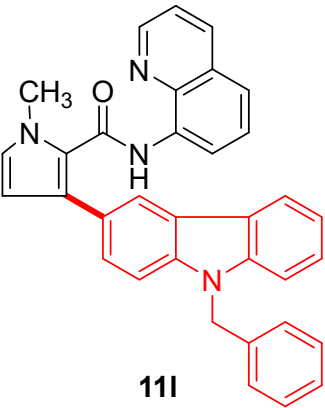
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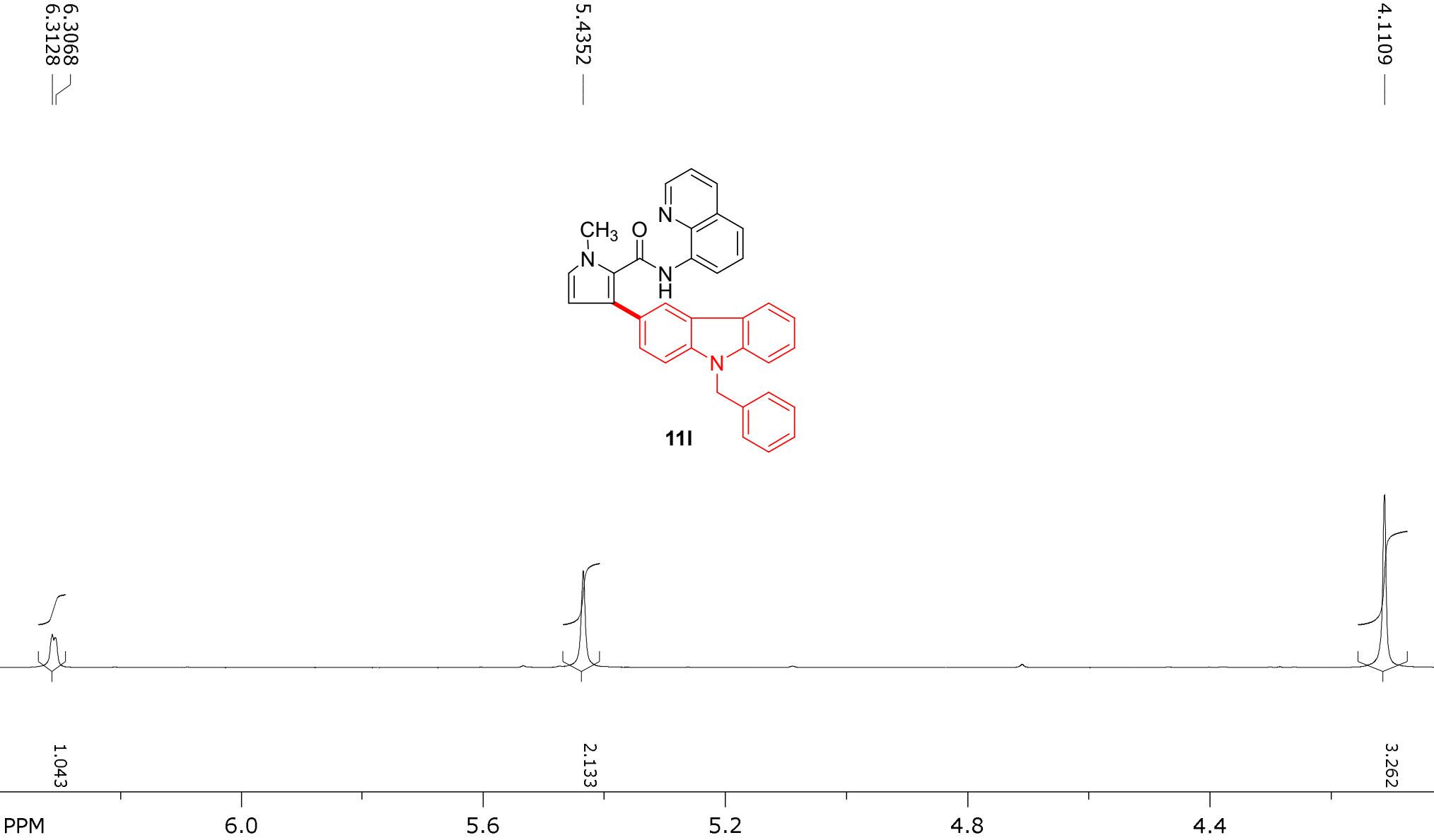
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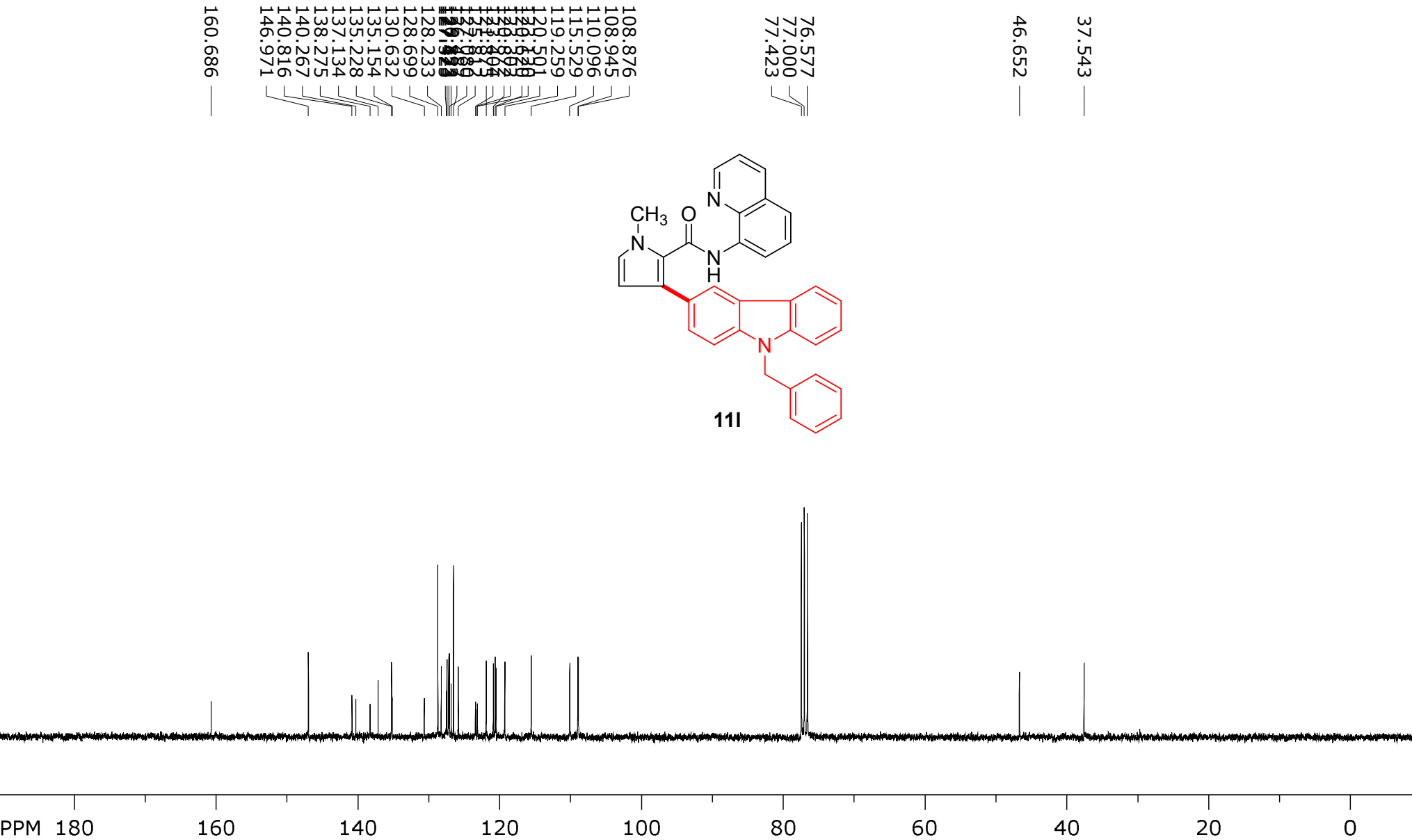
¹H

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SpinWorks 4: RD 631
1H





160.686

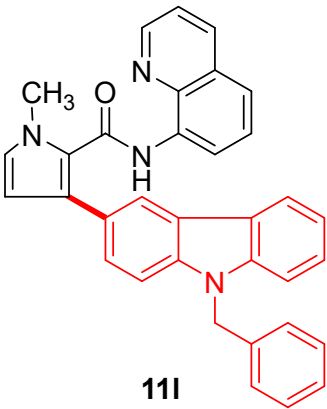
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140.267
140.816

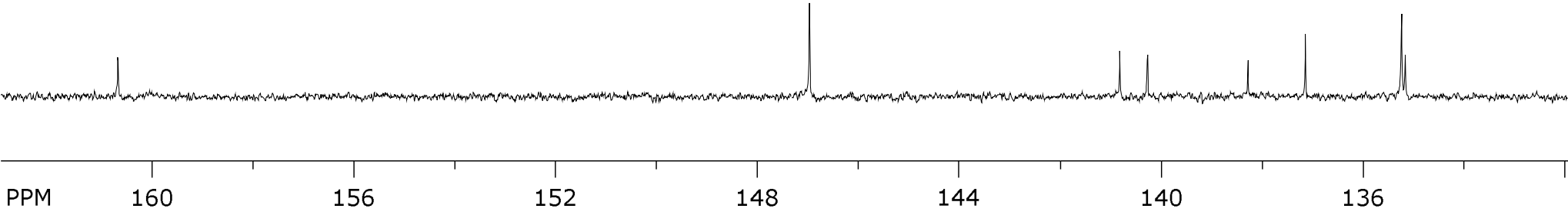
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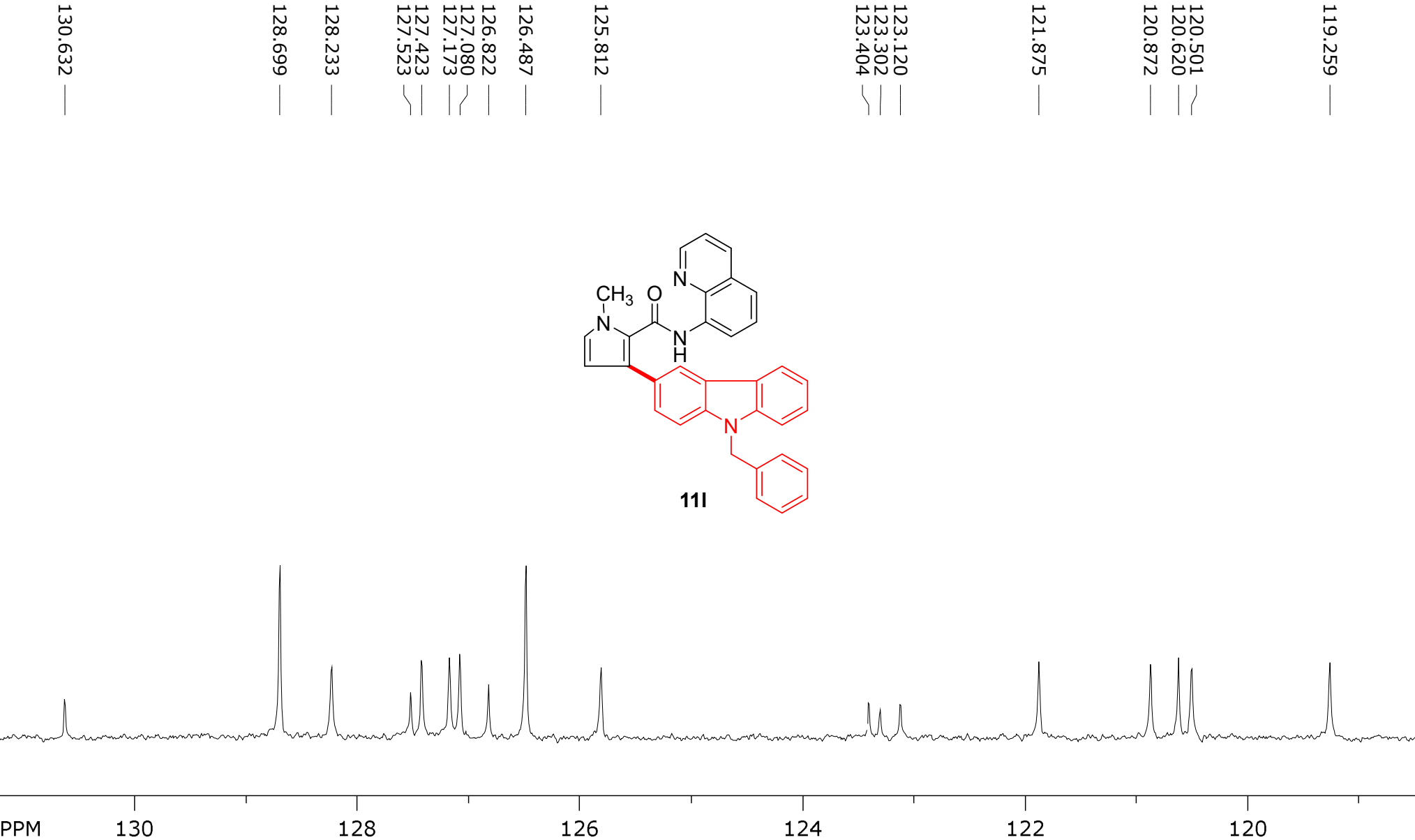
137.134

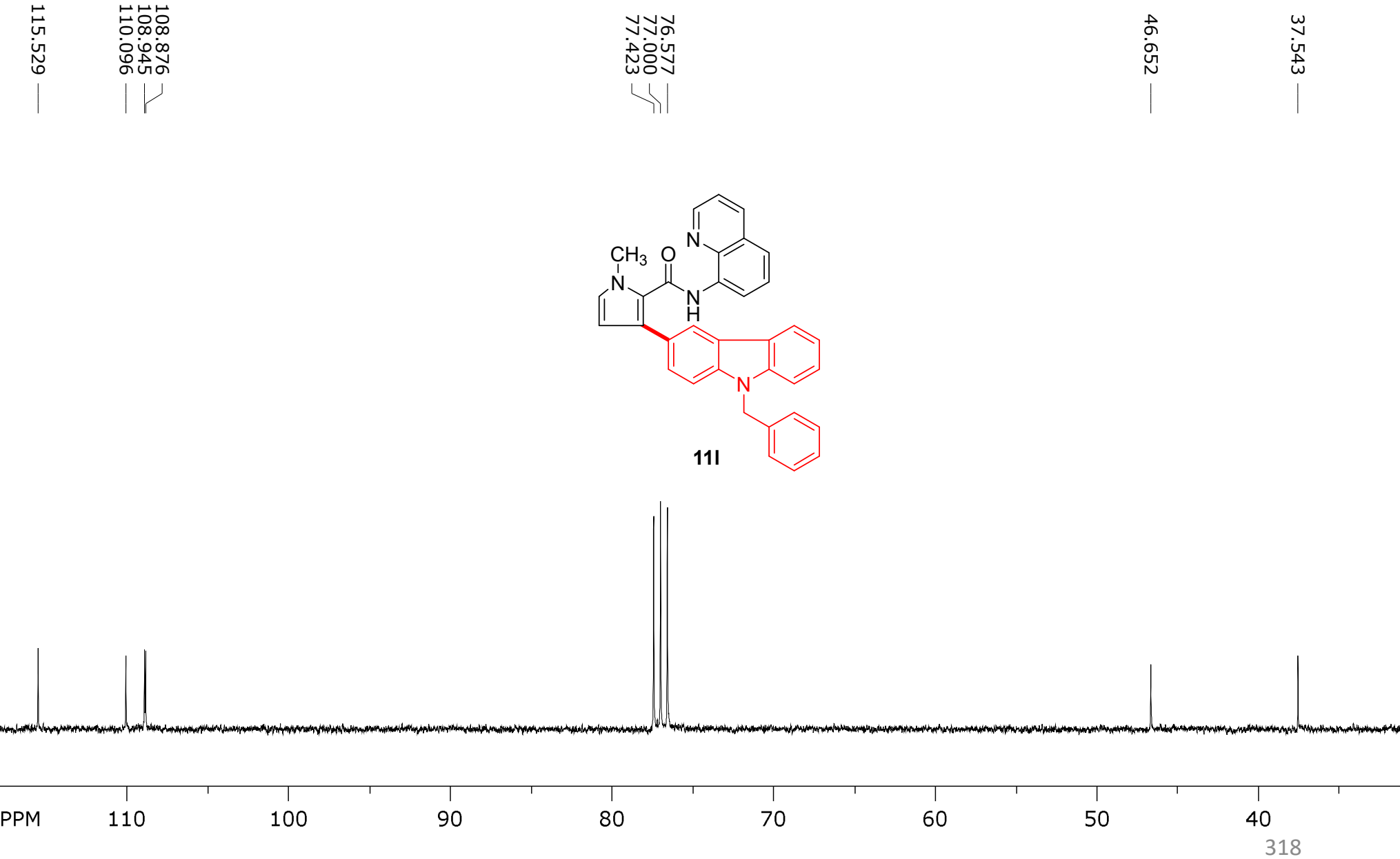
135.154
135.228



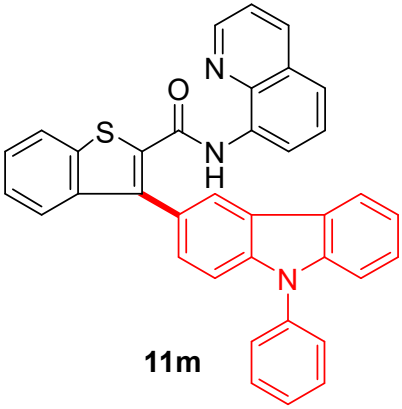
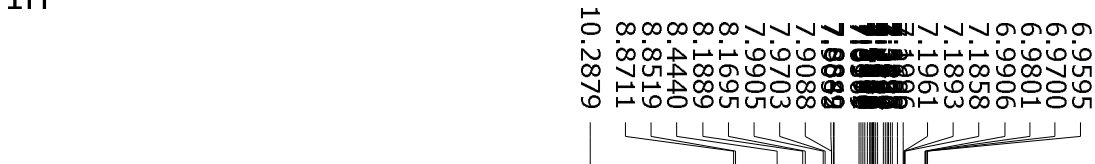
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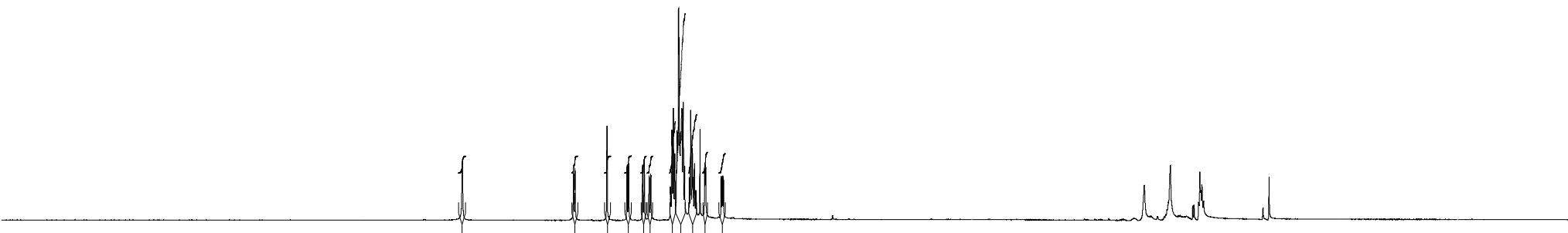




SpinWorks 4: RD 622
1H



11m



1.000
1.011
0.999
1.015
1.091
1.152
1.133
1.133
1.133
1.133

PPM 12 8 4 0 319

SpinWorks 4: RD 622

¹H

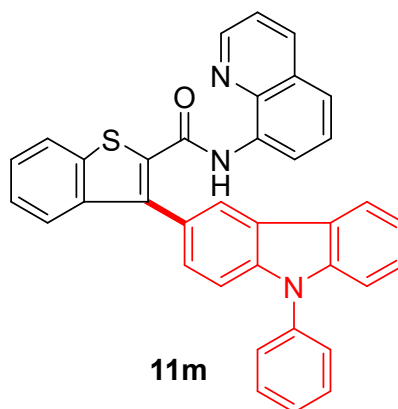
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8.8519
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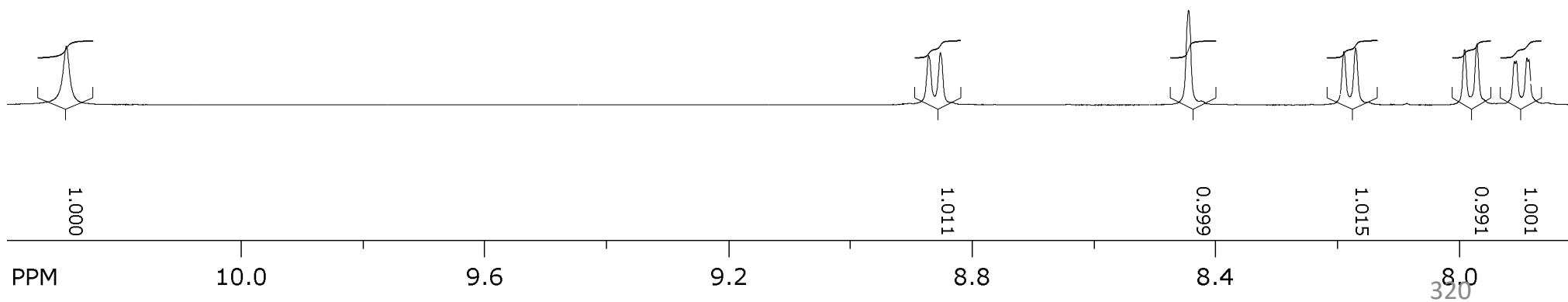
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8.1889

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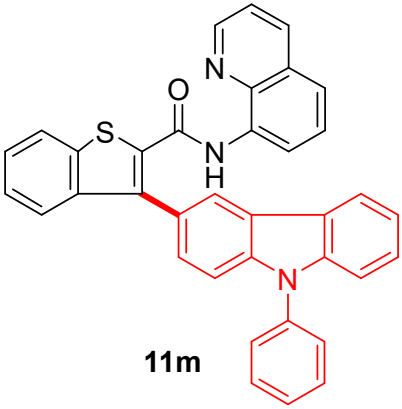
11m



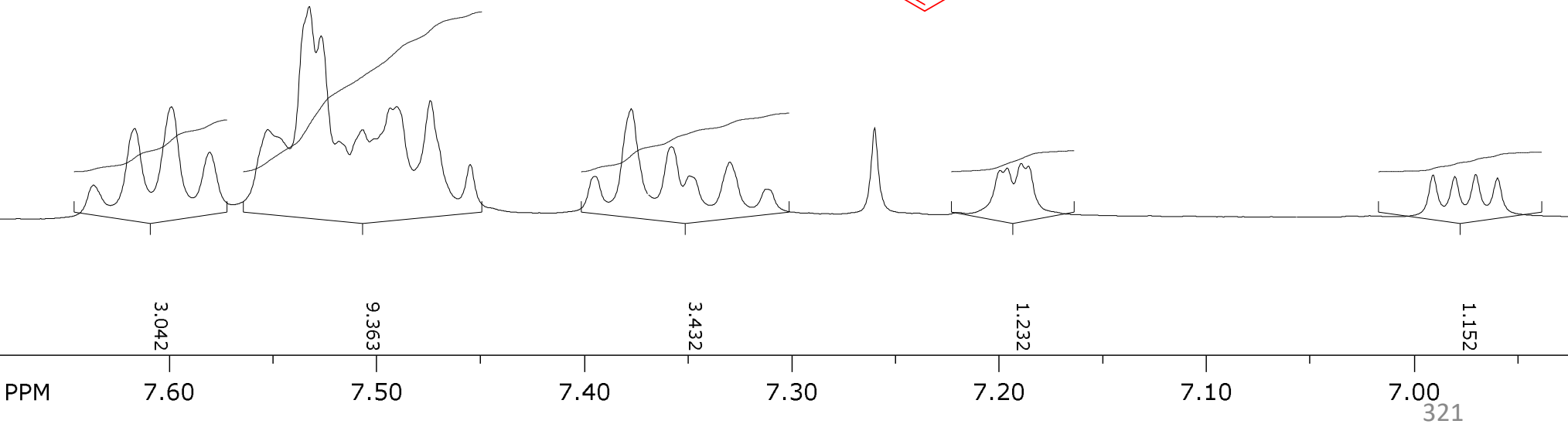
SpinWorks 4: RD 622

¹H

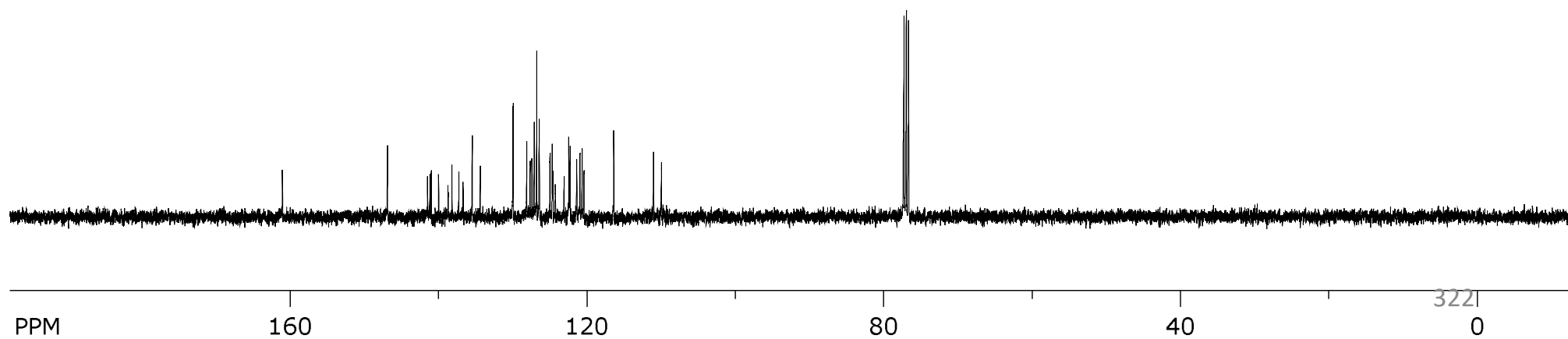
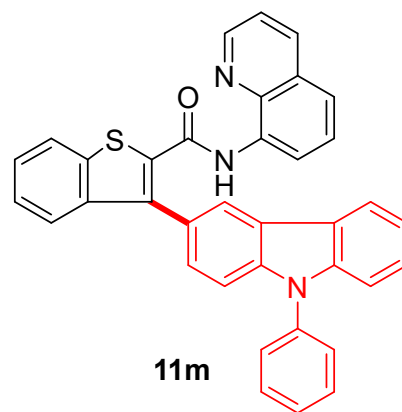
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—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



11m



SpinWorks 4: RD-622
13C



SpinWorks 4: RD-622
13C

161.146 —

146.969 —

141.074 —
141.247 —
141.565 —

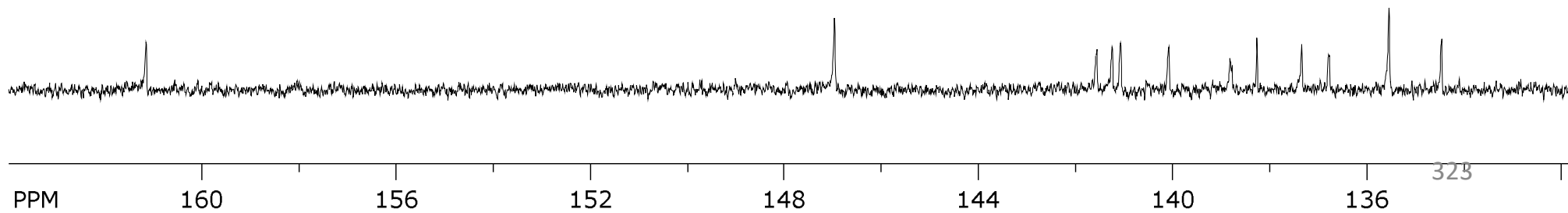
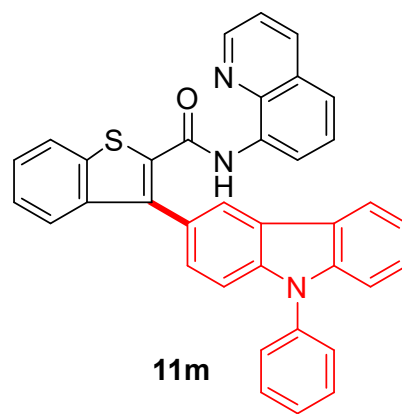
140.080 —

138.267 —
138.780 —
138.820 —

137.344 —
136.787 —

135.547 —

134.463 —



SpinWorks 4: RD-622
13C

130.047 —

126.490 —
126.847 —
127.194 —
127.485 —
127.738 —
128.186 —

124.361 —
124.649 —
124.749 —
125.056 —

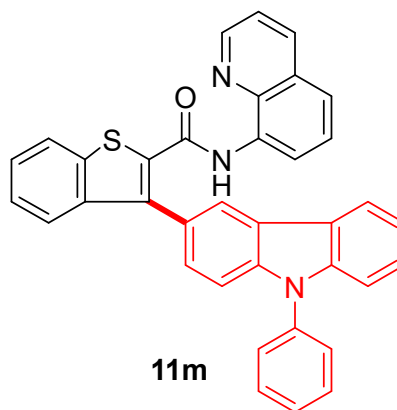
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122.353 —
122.512 —

121.451 —
120.478 —
120.717 —
121.019 —

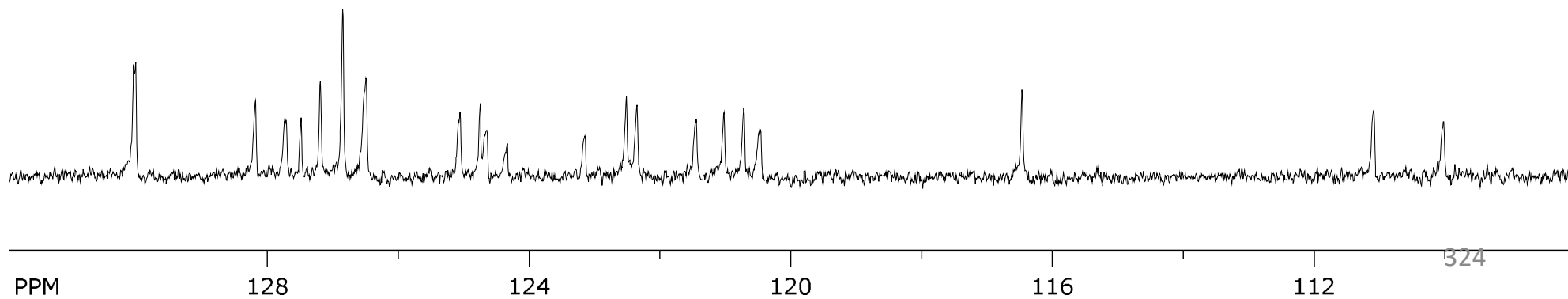
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111.084 —

110.010 —

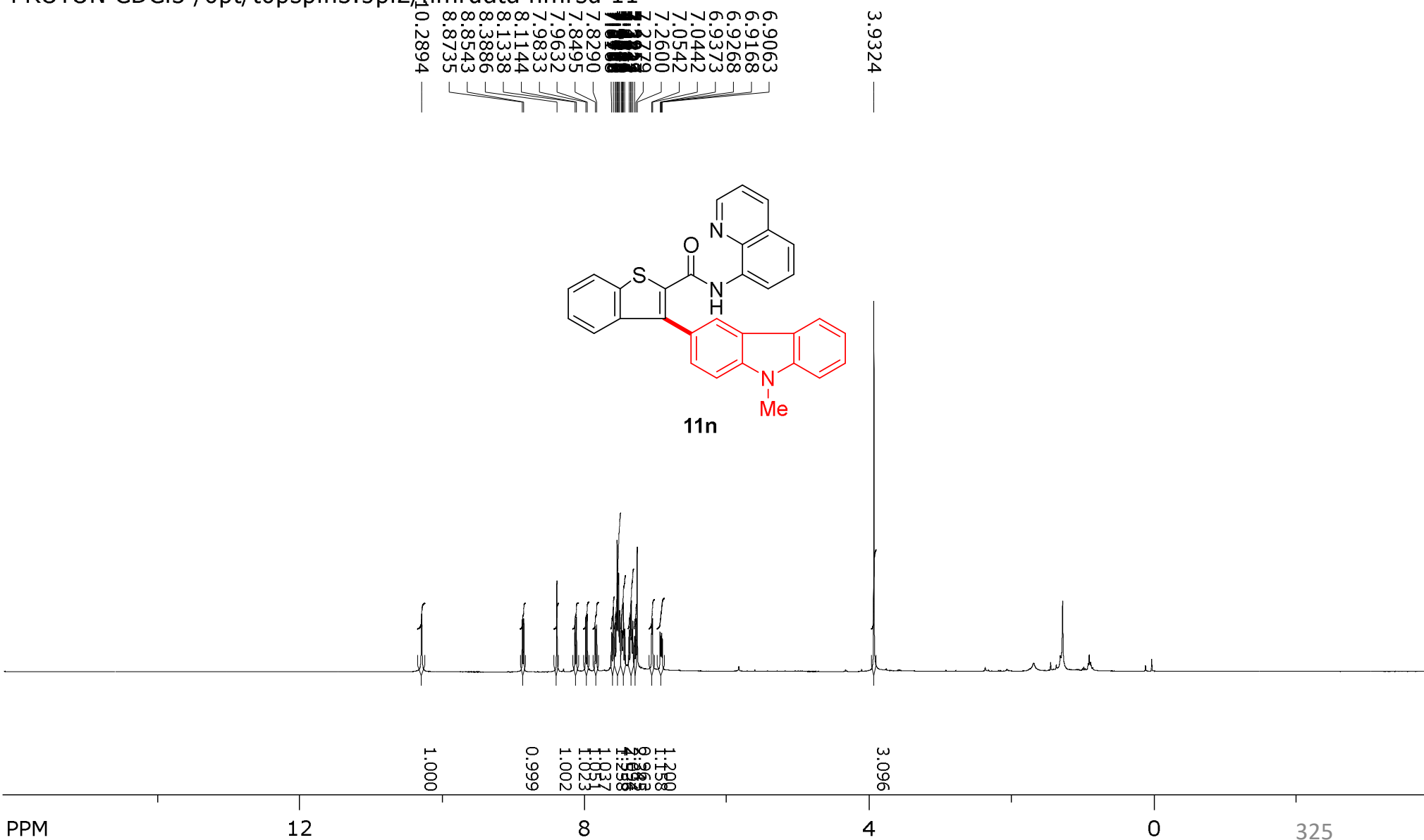


11m

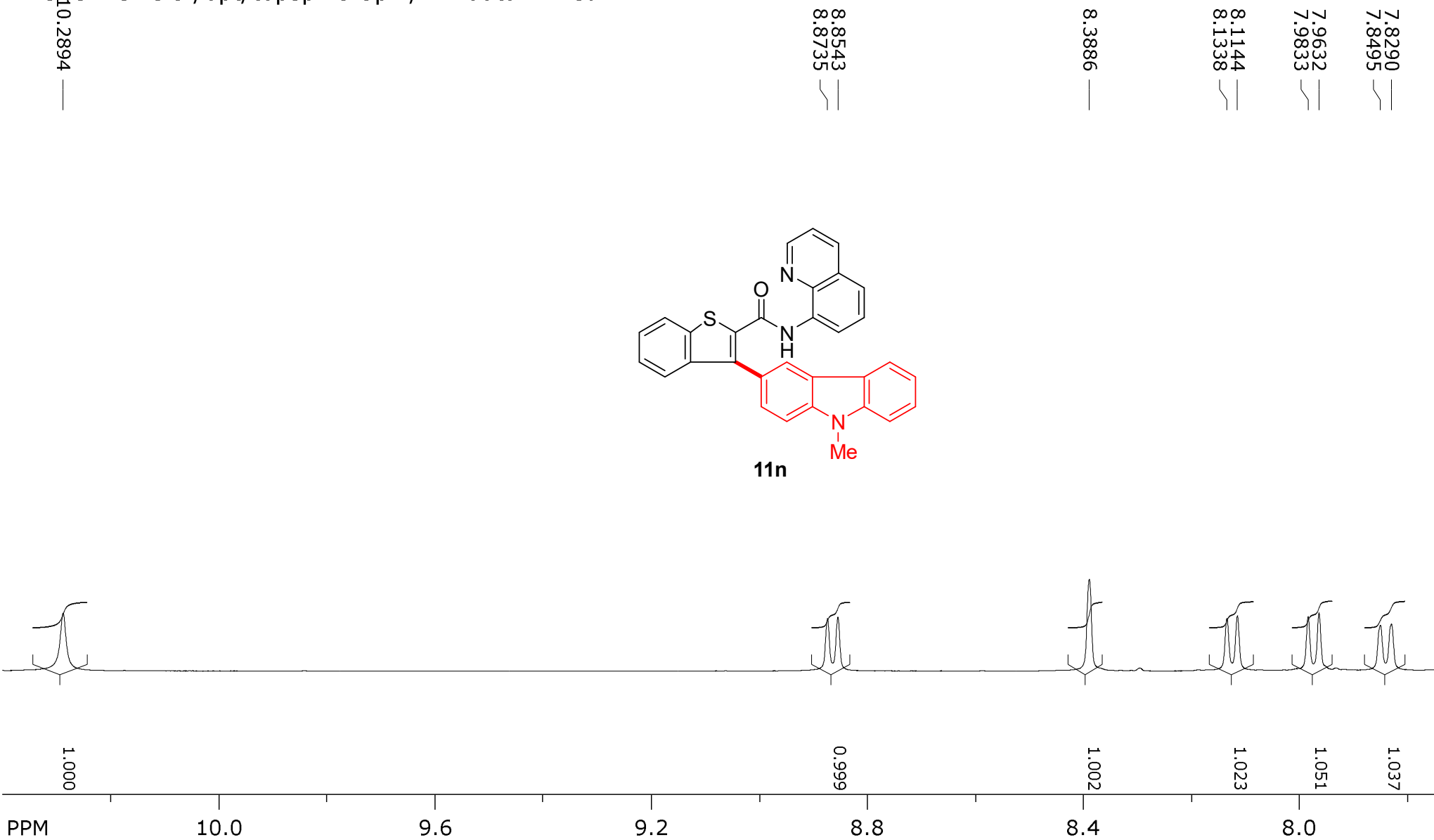


SpinWorks 4: RD 504

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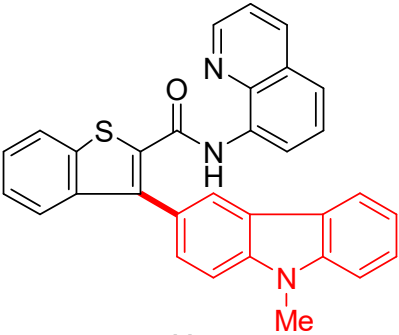


SpinWorks 4: RD 504
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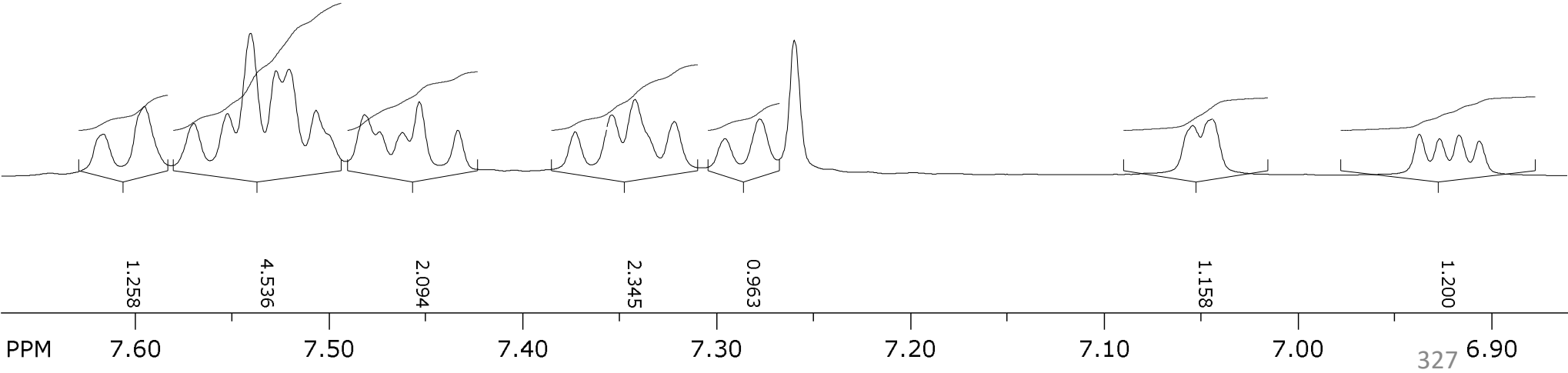


SpinWorks 4: RD 504
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

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7.5956 —
7.5700 —
7.5527 —
7.5407 —
7.5276 —
7.5208 —
7.5070 —
7.4819 —
7.4742 —
7.4623 —
7.4536 —
7.4337 —
7.3731 —
7.3541 —
7.3422 —
7.3219 —
7.2957 —
7.2779 —
7.2600 —
7.0442 —
7.0542 —
6.9373 —
6.9268 —
6.9168 —
6.9063 —

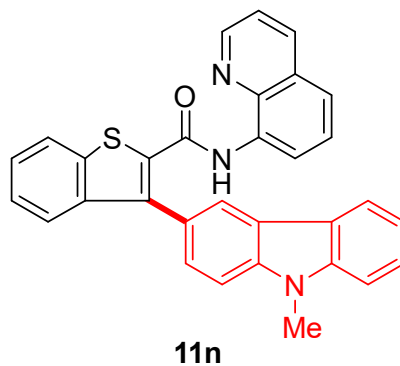
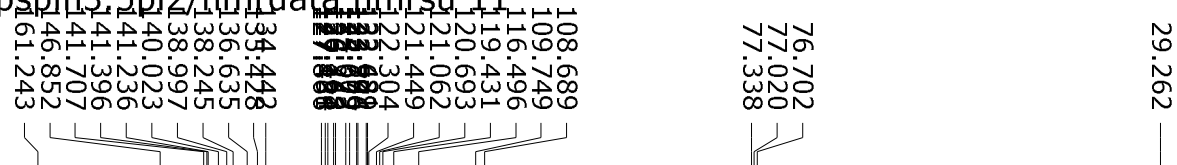


11n



SpinWorks 4: RD 504

C13CPD256 CDCl3 /opt/topspin3.5p2/nmrdata/nmr_su_11



PPM

160

120

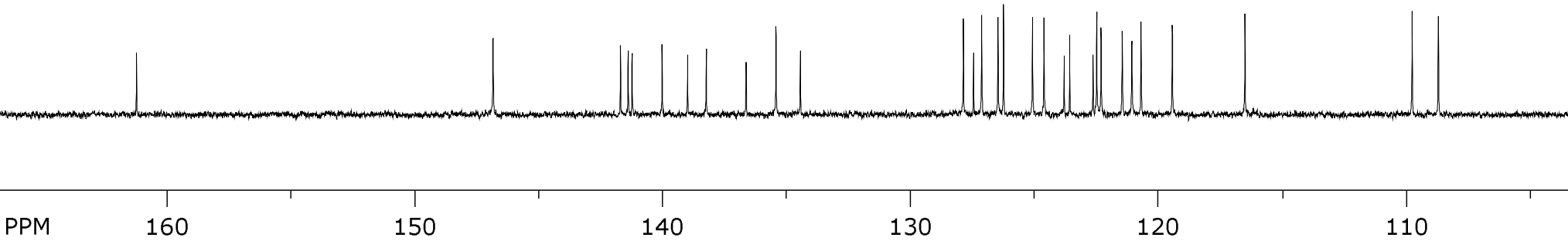
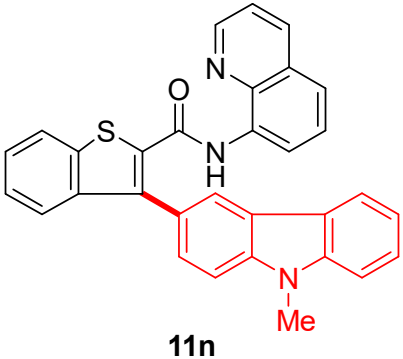
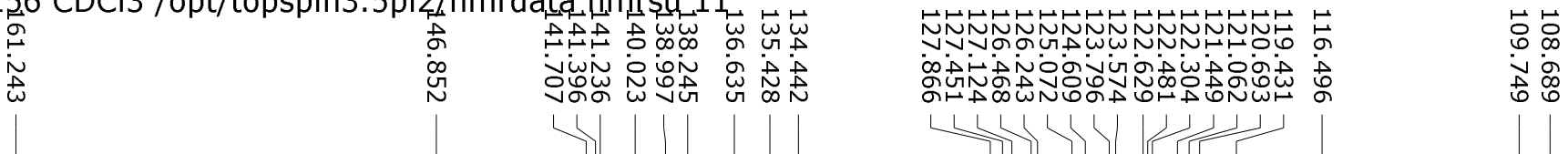
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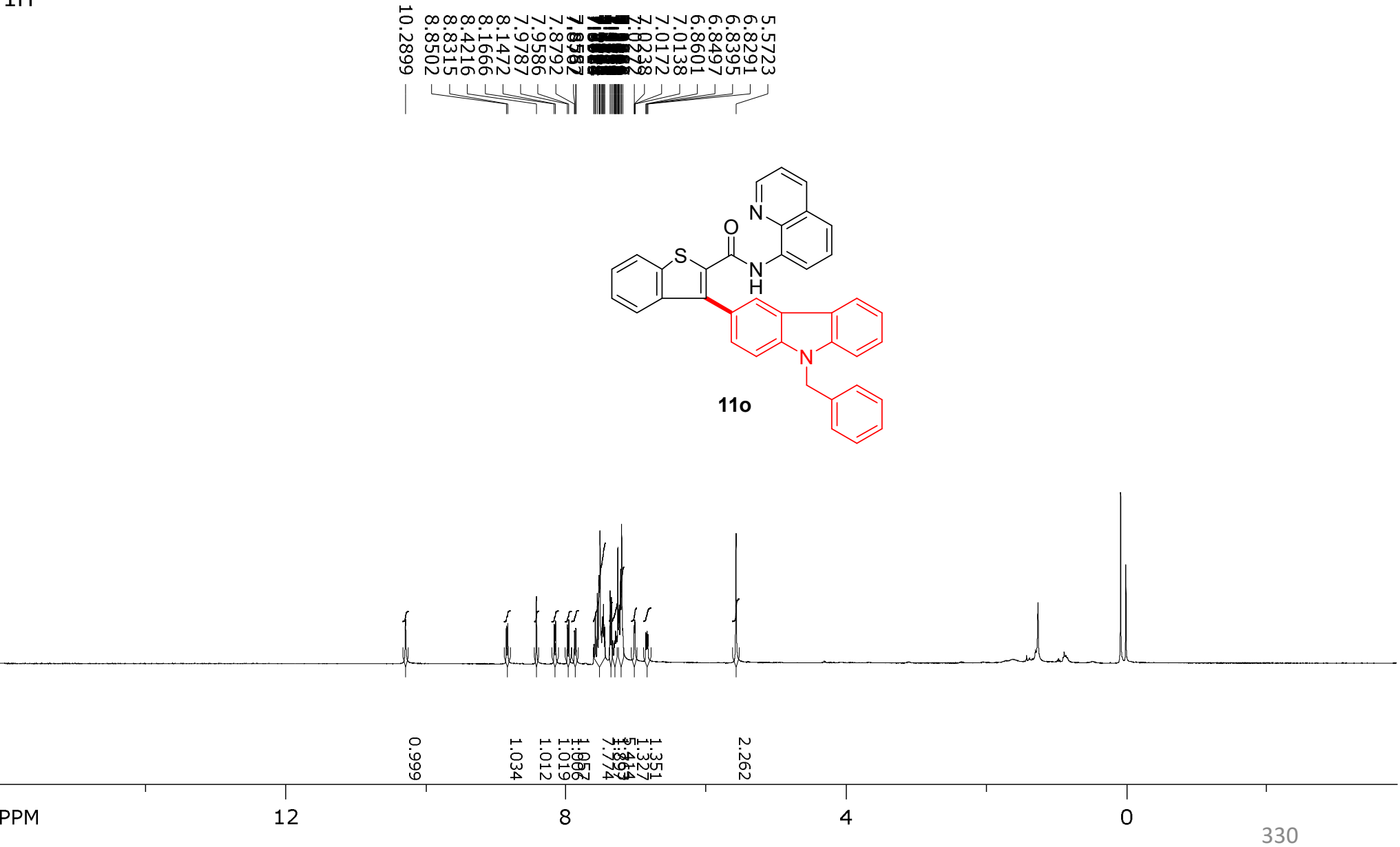
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328

SpinWorks 4: RD 504
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu_11



SpinWorks 4: RD 625 REP 1
1H



SpinWorks 4: RD 625 REP 1

¹H

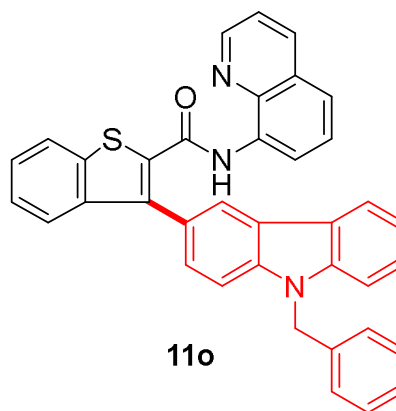
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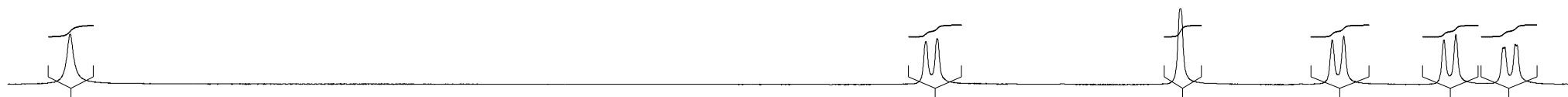
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8.1472
8.1666

7.8557
7.8587
7.8762
7.8792
7.9586
7.9787



11o



0.999

1.034

1.012

1.019

1.006

1.057

PPM

10.0

9.6

9.2

8.8

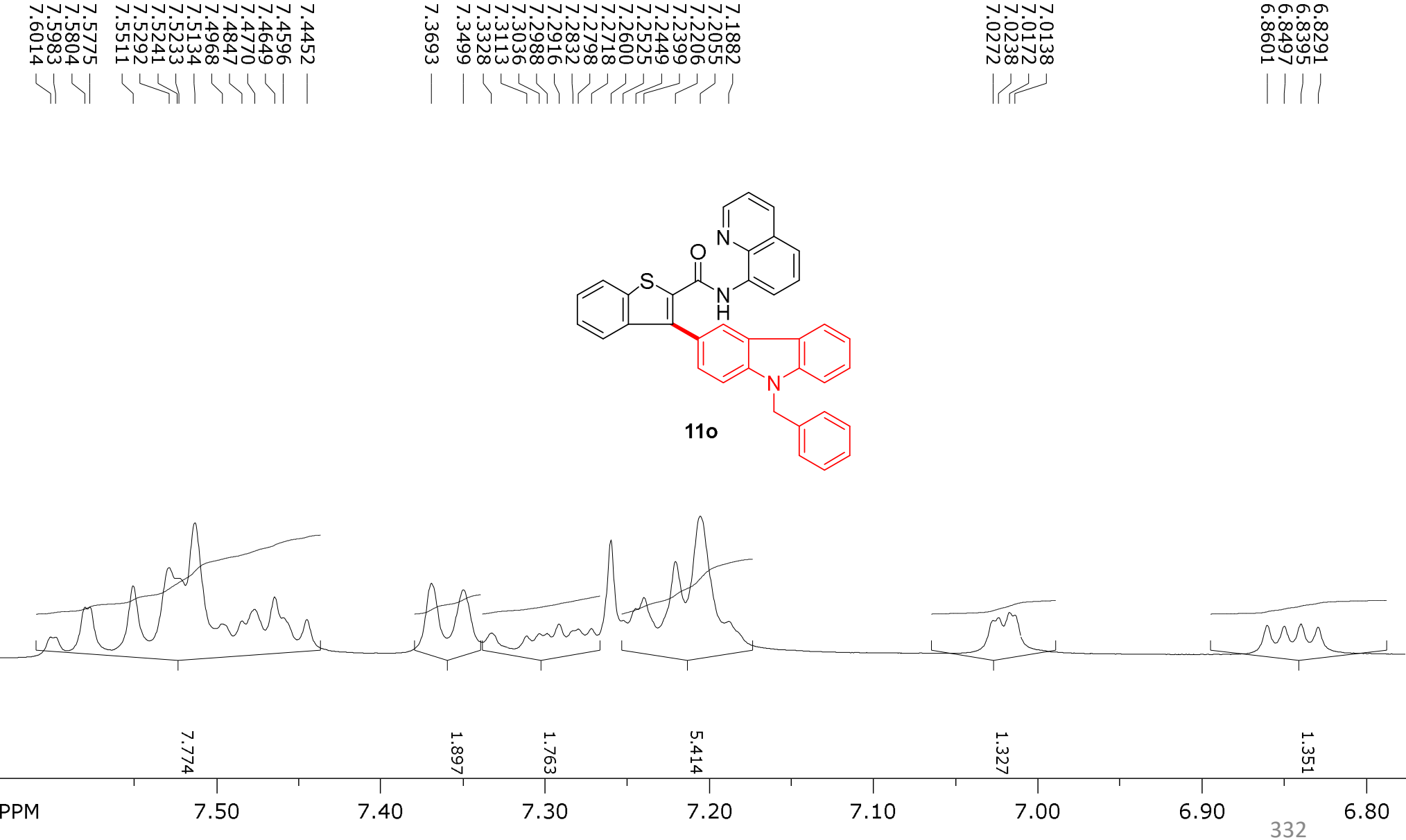
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331

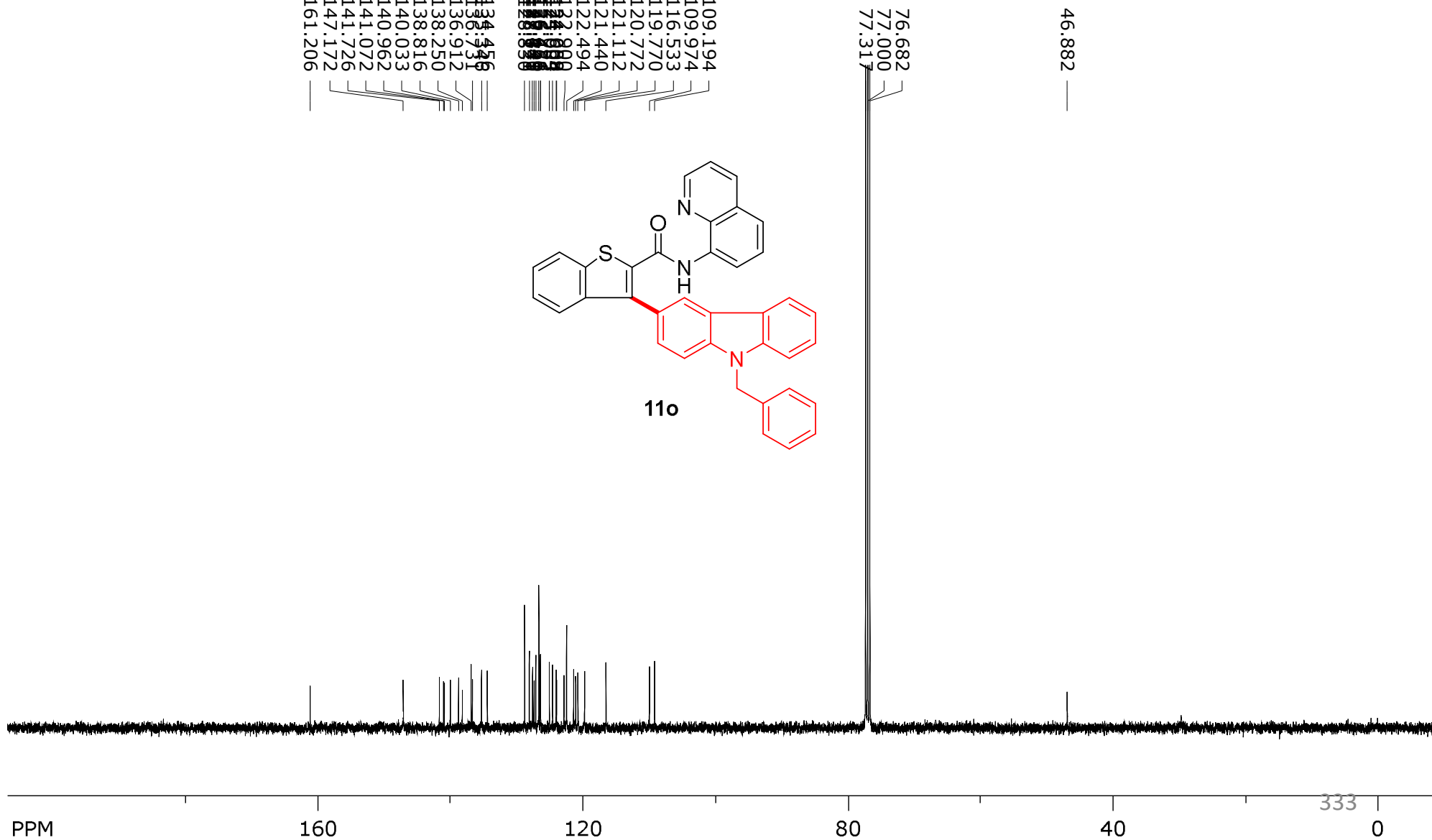
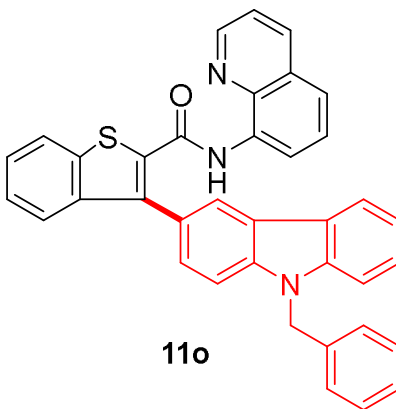
SpinWorks 4: RD 625 REP 1

¹H



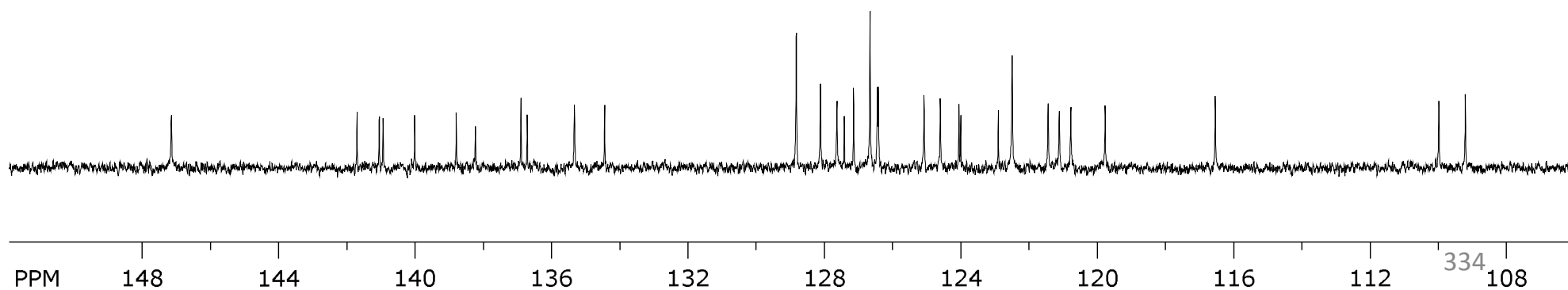
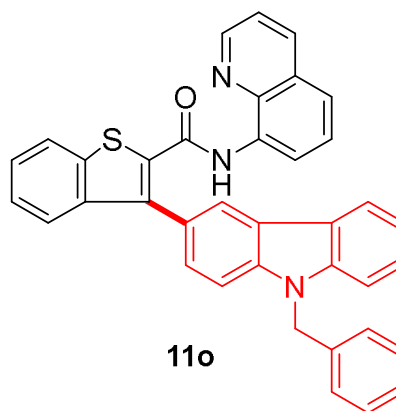
SpinWorks 4: RD-625
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128.898
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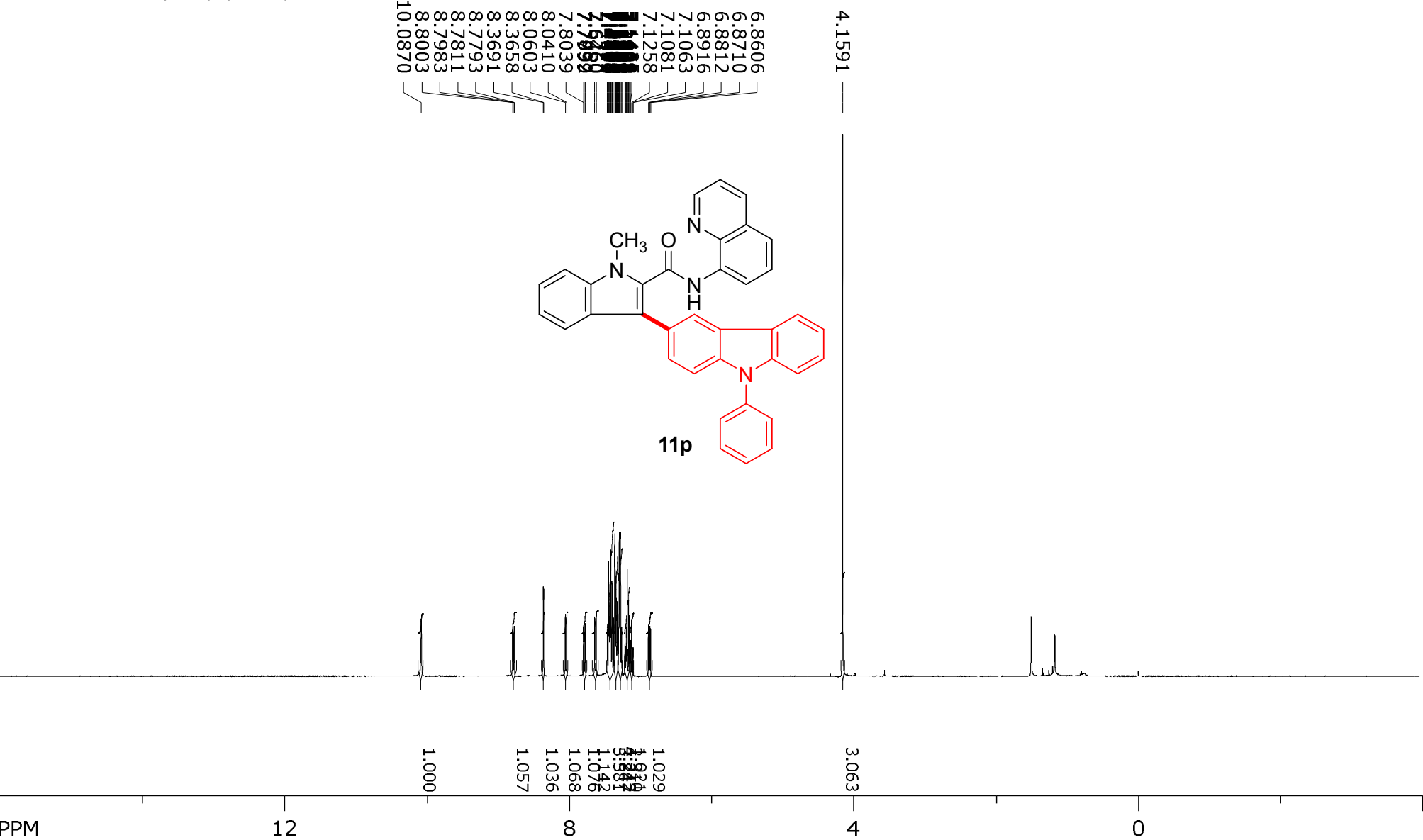


SpinWorks 4: RD-625
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

147.172	141.726	140.962	140.033	138.816	136.912	136.731	135.346	134.456	128.830	128.121	127.640	127.421	127.149	126.668	126.456	126.421	125.085	124.604	124.059	124.008	122.900	122.494	121.440	121.112	120.772	119.770	116.533	109.974	109.194
---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------



SpinWorks 4: RD-915
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



SpinWorks 4: RD-915

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 26

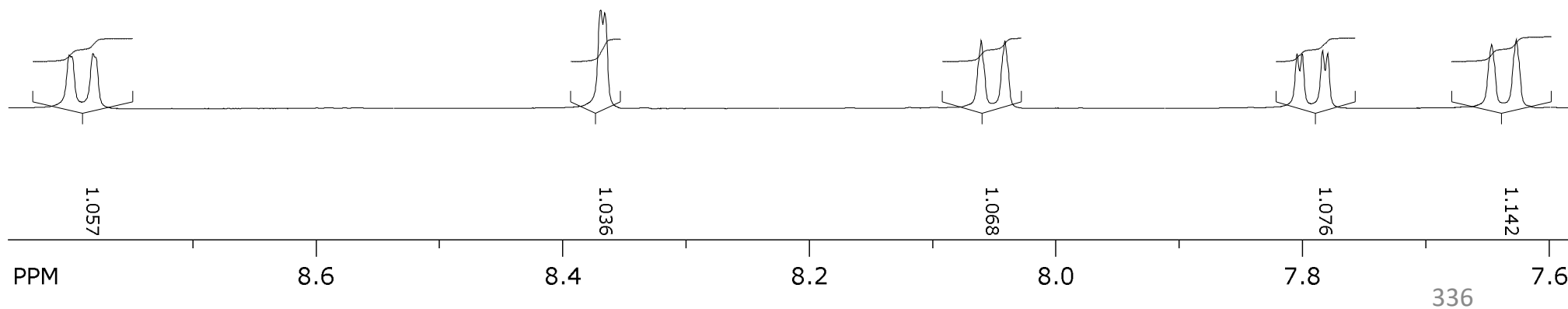
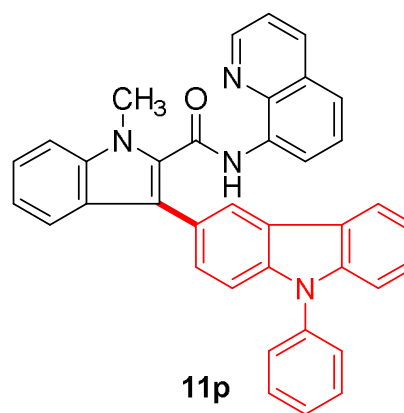
8.7793
8.7811
8.7983
8.8003

8.3658
8.3691

8.0410
8.0603

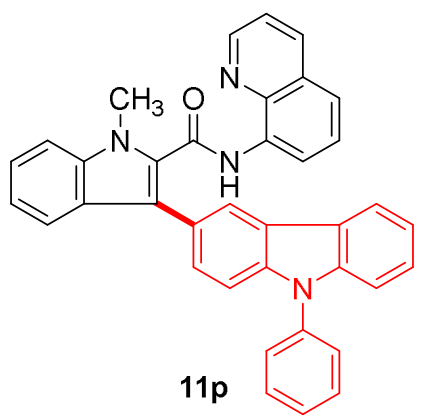
7.7792
7.7832
7.7999
7.8039

7.6260
7.6460

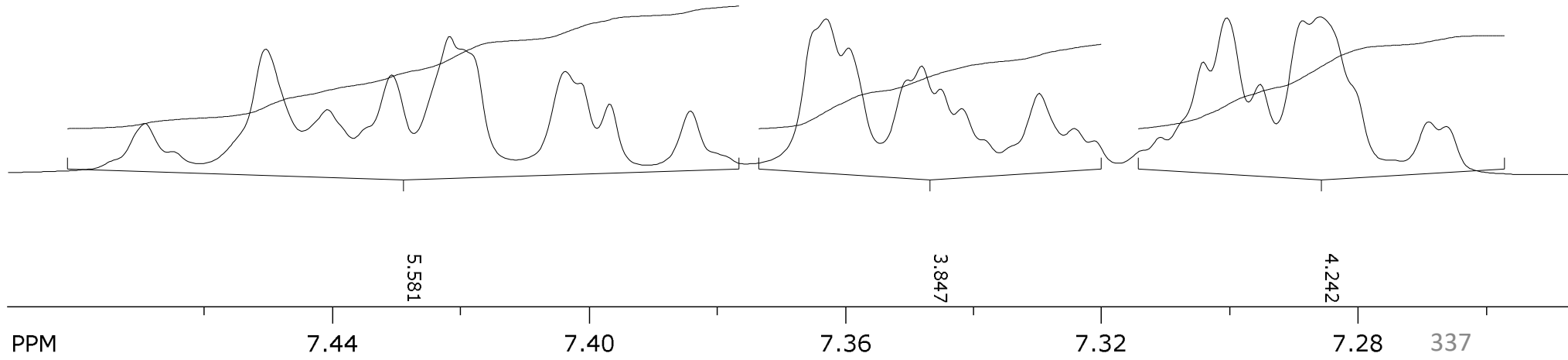


SpinWorks 4: RD-915
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

7.4693	7.4505	7.4408	7.4308	7.4218	7.4037	7.3968	7.3842	7.3630	7.3595	7.3503	7.3481	7.3451	7.3418	7.3387	7.3297	7.3242	7.3212	7.3108	7.3005	7.2953	7.2886	7.2859	7.2689	7.2662
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



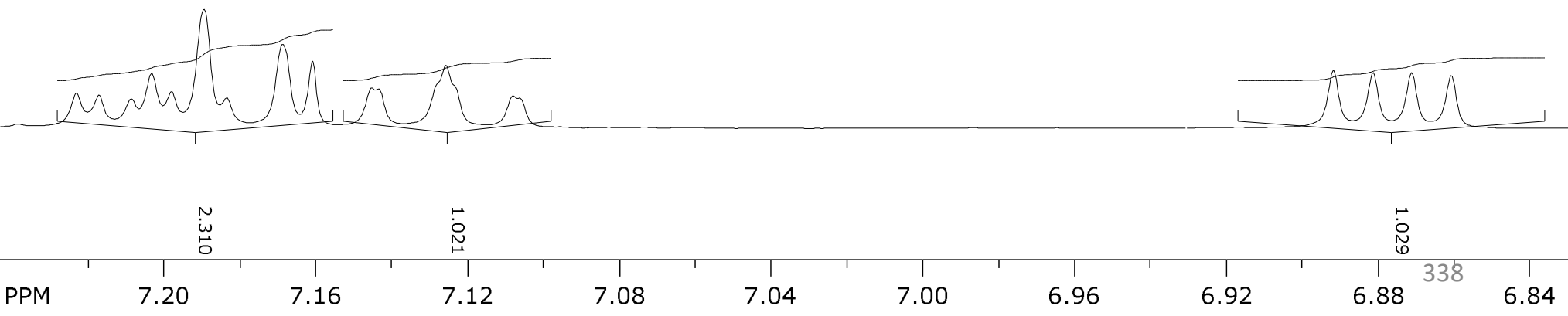
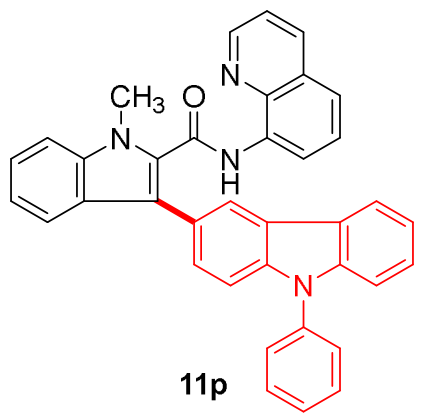
11p



SpinWorks 4: RD-915
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26

7.1063	7.1081	7.1258	7.1435	7.1453	7.1609	7.1689	7.1835	7.1896	7.1981	7.2034	7.2087	7.2173	7.2232
—	—	—	—	—	—	—	—	—	—	—	—	—	—

6.8606	6.8710	6.8812	6.8916
—	—	—	—



C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

12
13
14
15
16

109.781
110.037
110.357
115.891
120.092
120.513
120.596
120.944
121.169
121.391
121.609
121.834
122.065
122.294
122.529
122.764
123.000
123.234
123.470
123.707
123.944
124.182
124.420
124.658
124.896
125.134
125.372
125.610
125.848
126.086
126.324
126.562
126.800
127.038
127.276
127.514
127.752
127.990
128.228
128.466
128.704
128.942
129.180
129.418
129.656
129.894
130.132
130.370
130.608
130.846
131.084
131.322
131.560
131.798
132.036
132.274
132.512
132.750
132.988
133.226
133.464
133.702
133.940
134.178
134.416
134.654
134.892
135.130
135.368
135.606
135.844
136.082
136.320
136.558
136.796
137.034
137.272
137.510
137.748
137.986
138.224
138.462
138.700
138.938
139.176
139.414
139.652
139.890
140.128
140.366
140.604
140.842
141.080
141.318
141.556
141.794
142.032
142.270
142.508
142.746
142.984
143.222
143.460
143.698
143.936
144.174
144.412
144.650
144.888
145.126
145.364
145.602
145.840
146.078
146.316
146.554
146.792
147.030
147.268
147.506
147.744
147.982
148.220
148.458
148.696
148.934
149.172
149.410
149.648
149.886
150.124
150.362
150.600
150.838
151.076
151.314
151.552
151.790
152.028
152.266
152.504
152.742
152.980
153.218
153.456
153.694
153.932
154.170
154.408
154.646
154.884
155.122
155.360
155.598
155.836
156.074
156.312
156.550
156.788
157.026
157.264
157.502
157.740
157.978
158.216
158.454
158.692
158.930
159.168
159.406
159.644
159.882
160.120
160.358
160.596
160.834
161.072
161.310
161.548
161.786
162.024
162.262
162.500
162.738
162.976
163.214
163.452
163.690
163.928
164.166
164.404
164.642
164.880
165.118
165.356
165.594
165.832
166.070
166.308
166.546
166.784
167.022
167.260
167.498
167.736
167.974
168.212
168.450
168.688
168.926
169.164
169.402
169.640
169.878
170.116
170.354
170.592
170.830
171.068
171.306
171.544
171.782
172.020
172.258
172.496
172.734
172.972
173.210
173.448
173.686
173.924
174.162
174.400
174.638
174.876
175.114
175.352
175.590
175.828
176.066
176.30

161.117

147.114

140.933

138.230
140.564

138.55/138.700

135.470

134.770

129.454
129.837

129.065

H-F-H
 N-D-N
 O-D-O
 - - -
 H-S-H
 C-S-C
 O-S-O

...
...
...
...
...
...

120.944

120.513
120.596

120.092

115.891

110.357

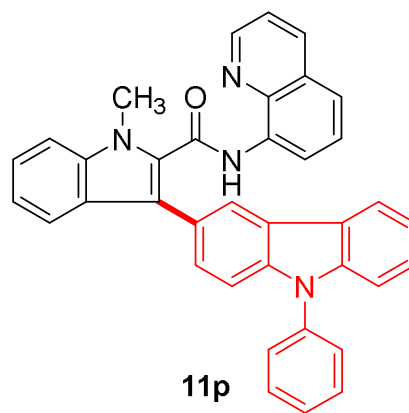
109.781
110.037

76.702
77.020
77.338

77.338

77.020

32.042 —



PPM

160

120

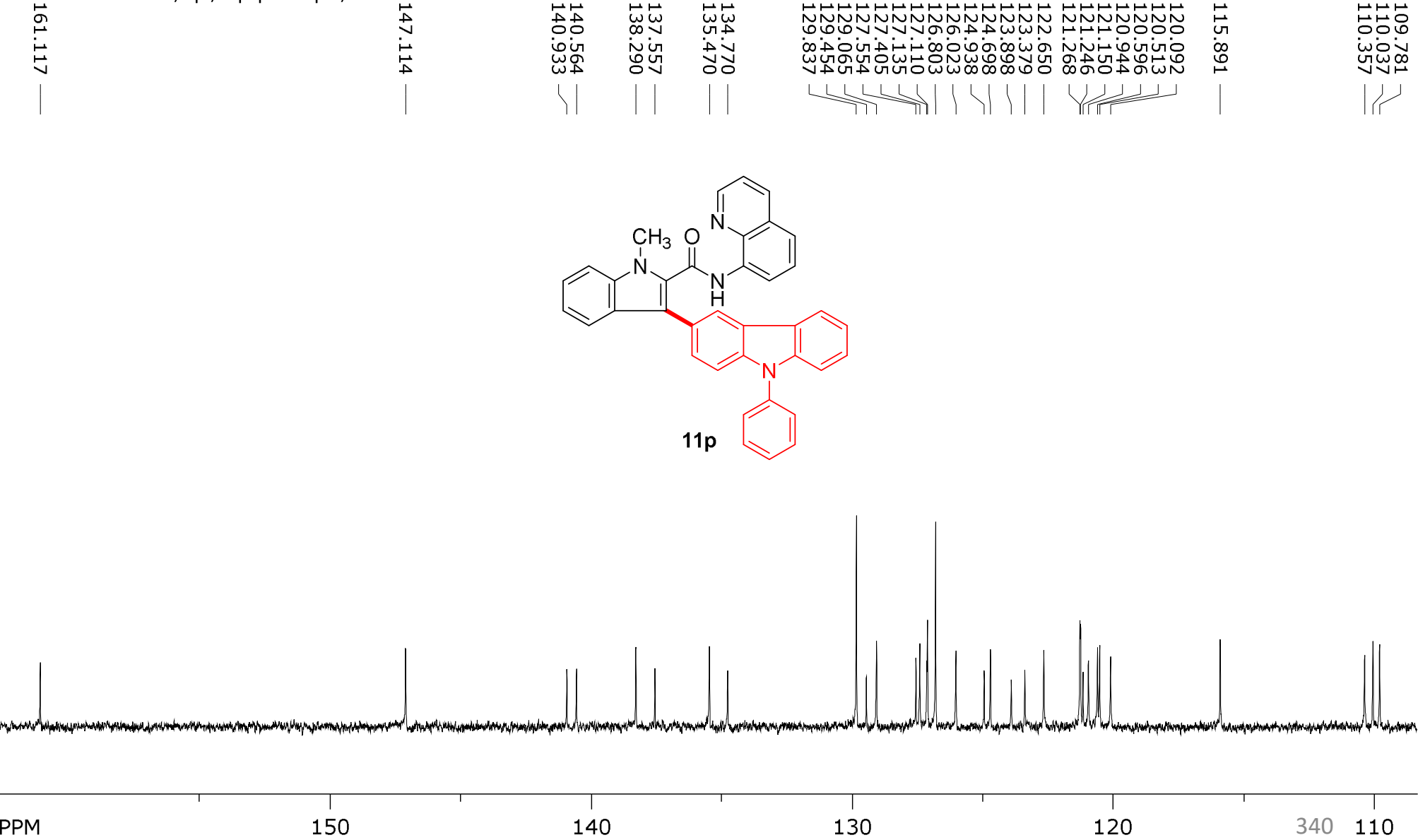
80

40

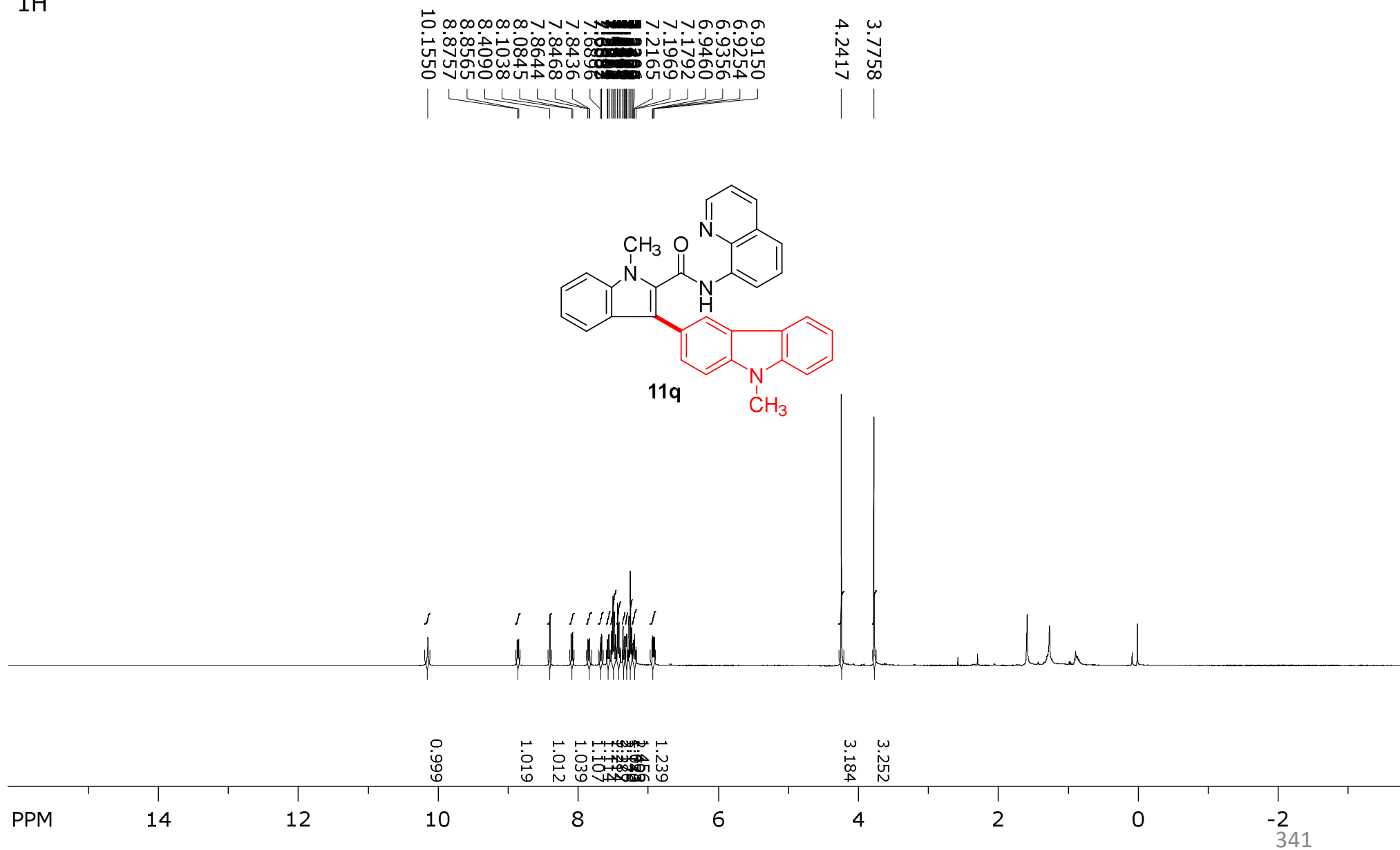
$$\begin{array}{r} 339 \\ 0 \end{array}$$

C

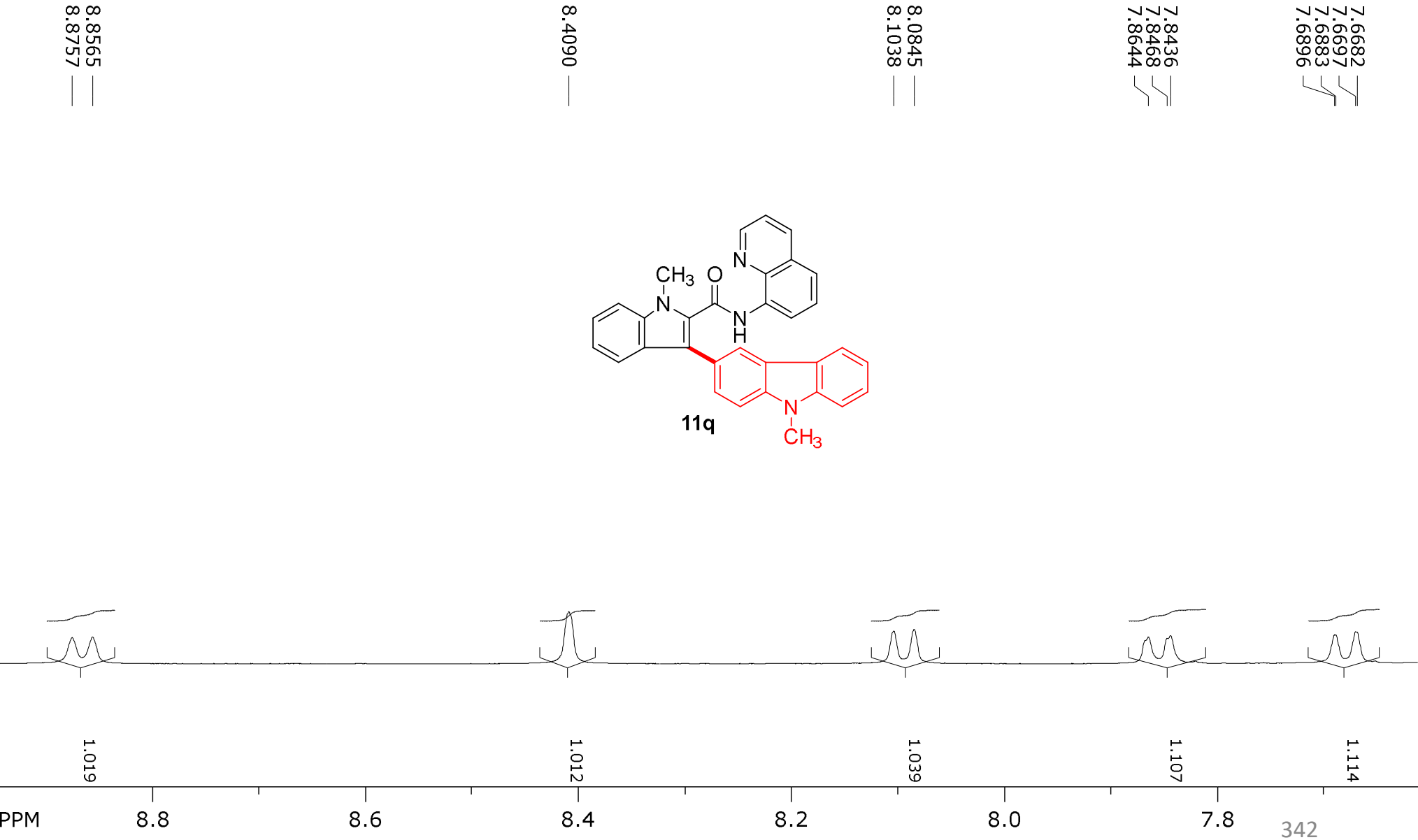
SpinWorks 4: RD 915
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



SpinWorks 4: RD 613
1H

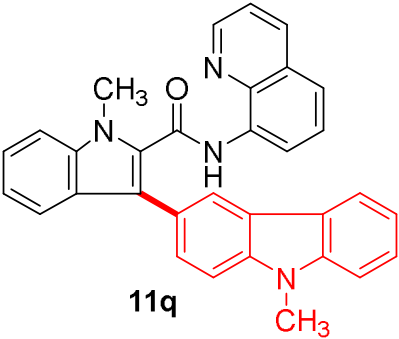


SpinWorks 4: RD 613
1H

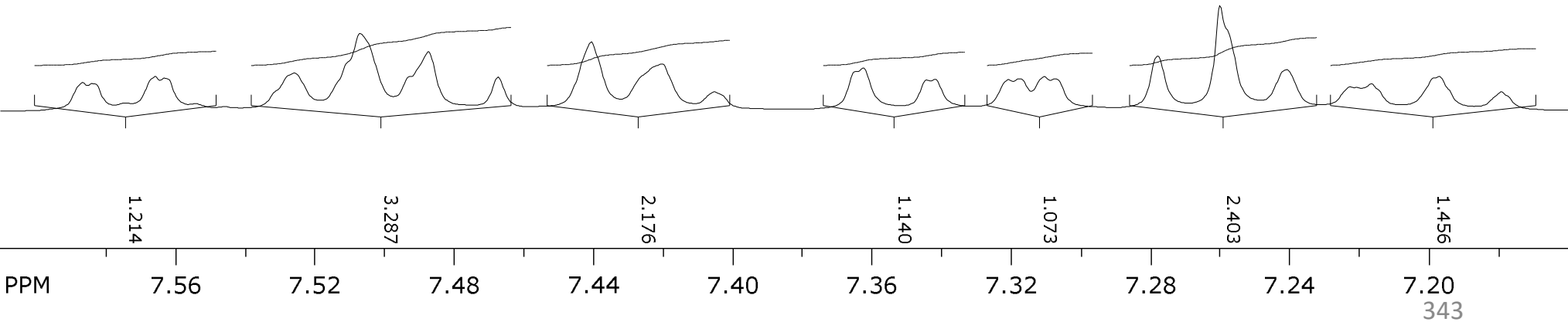


SpinWorks 4: RD 613
1H

7.1792 —
7.1969 —
7.2165 —
7.2206 —
7.2227 —
7.2409 —
7.2600 —
7.2779 —
7.3074 —
7.3105 —
7.3176 —
7.3208 —
7.3419 —
7.3443 —
7.3625 —
7.3647 —
7.4054 —
7.4203 —
7.4407 —
7.4675 —
7.4875 —
7.5072 —
7.5261 —
7.5634 —
7.5661 —
7.5842 —
7.5869 —

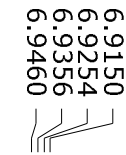


11q



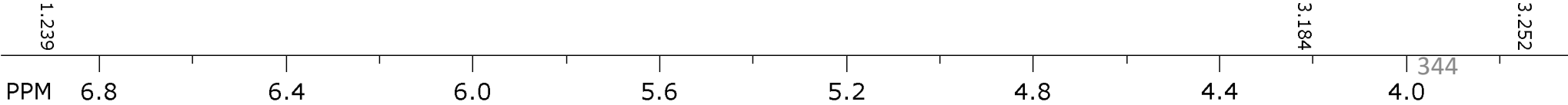
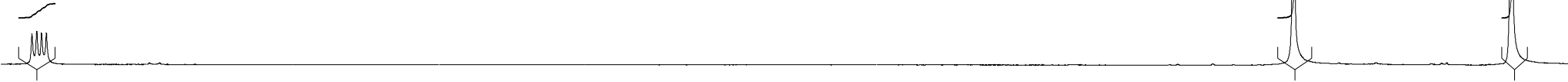
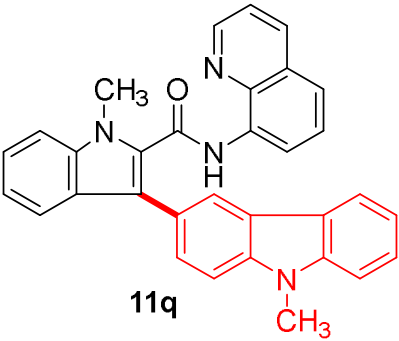
SpinWorks 4: RD 613

¹H

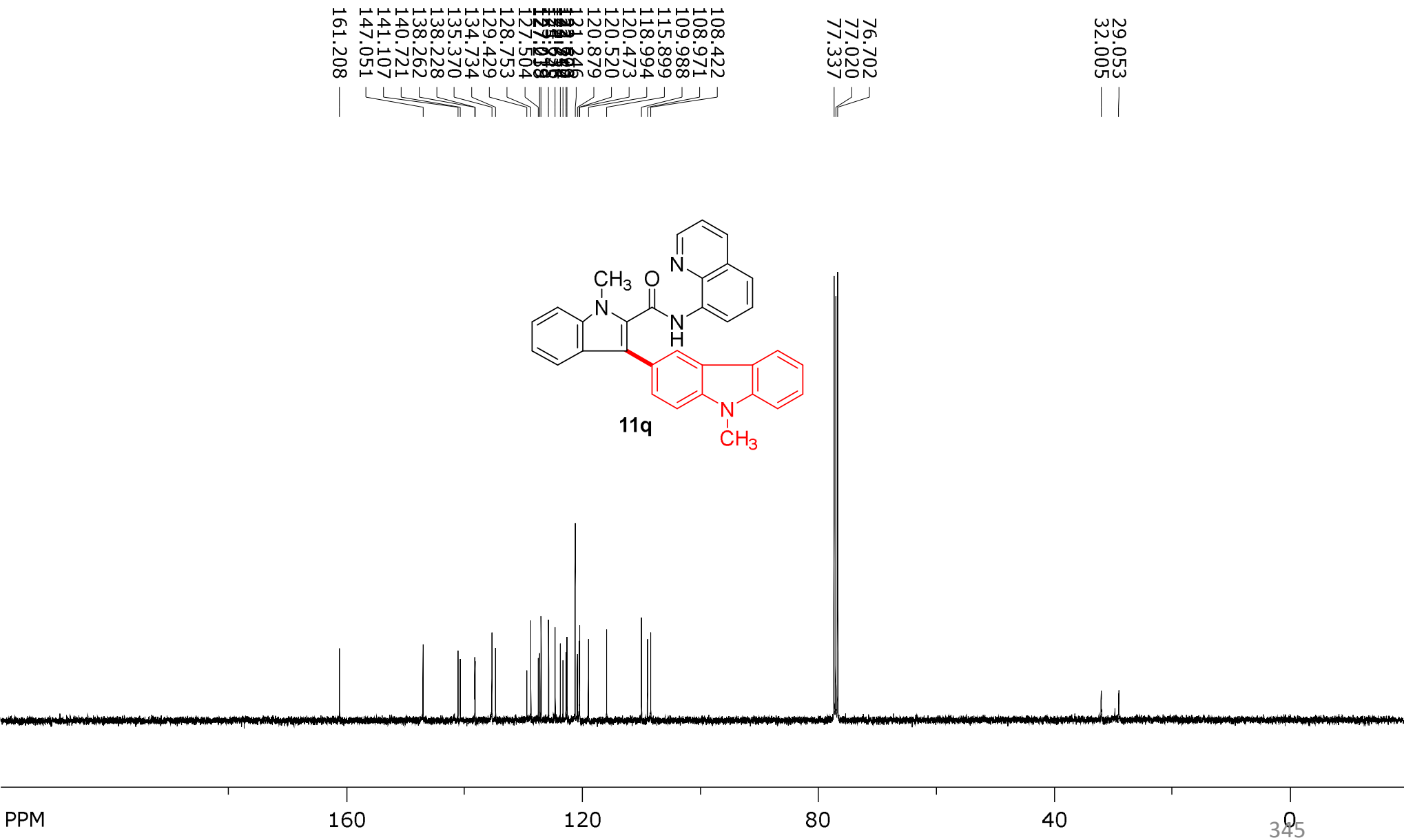


4.2417

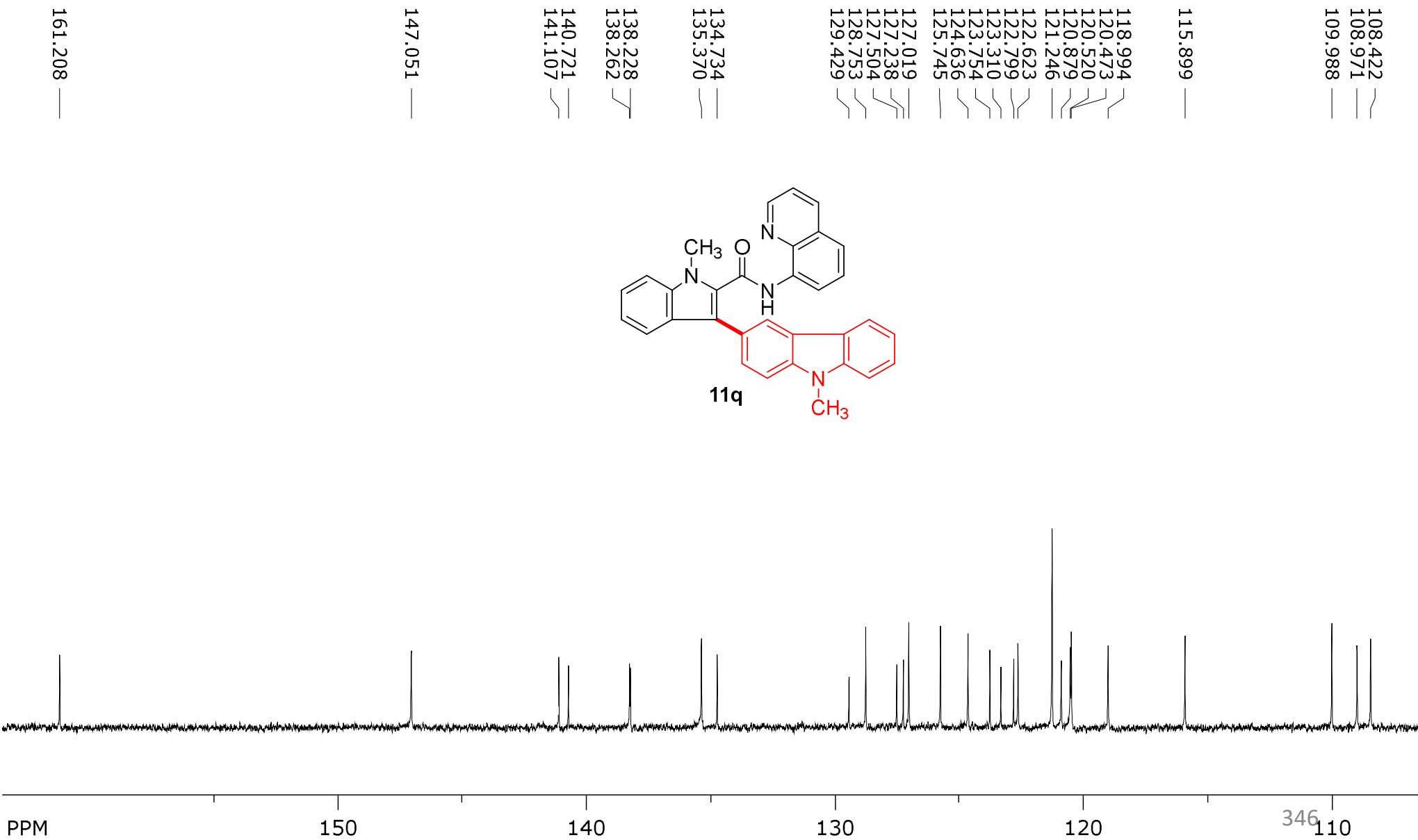
3.7758



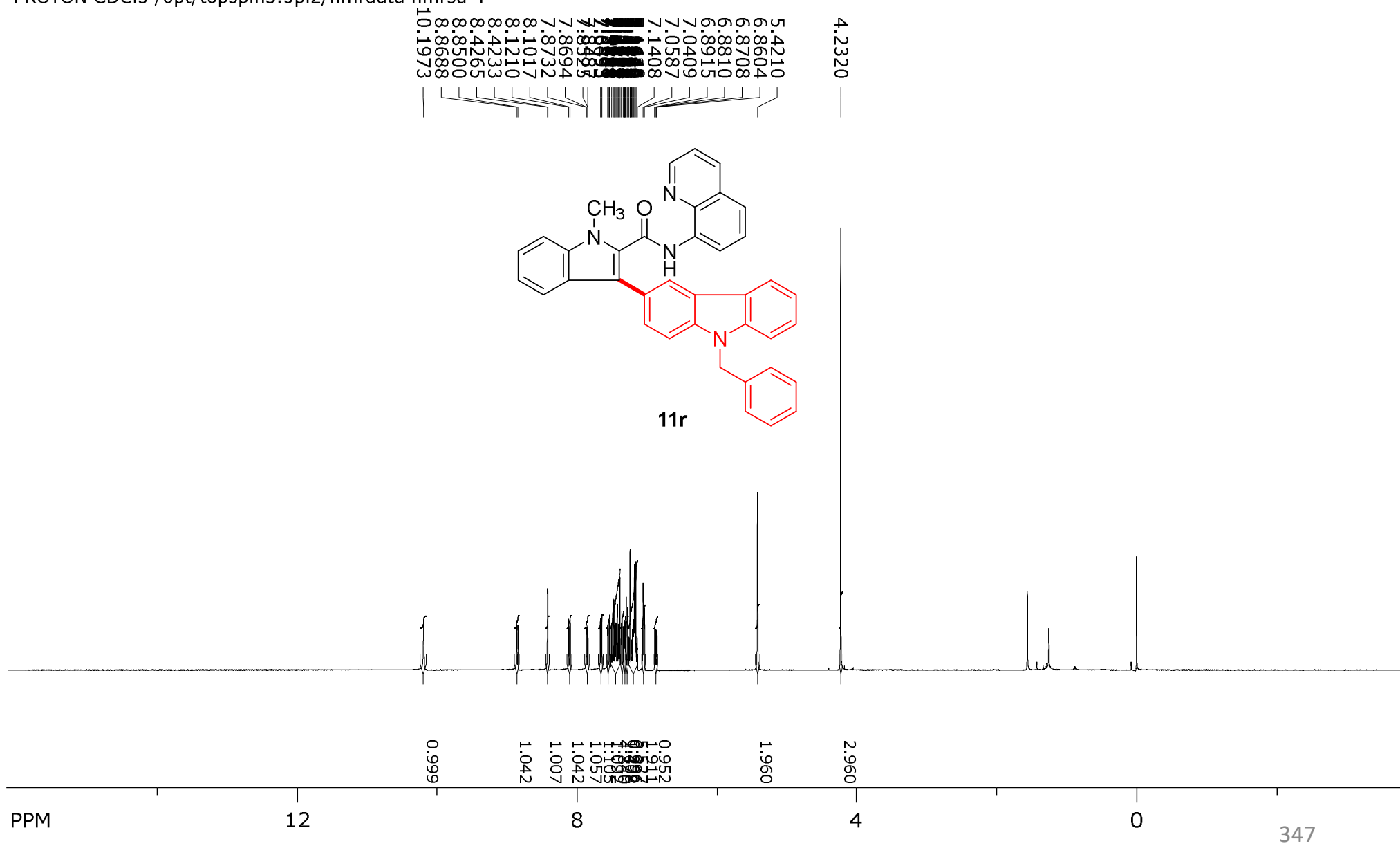
SpinWorks 4: RD 613



SpinWorks 4: RD 613



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: RD 898
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

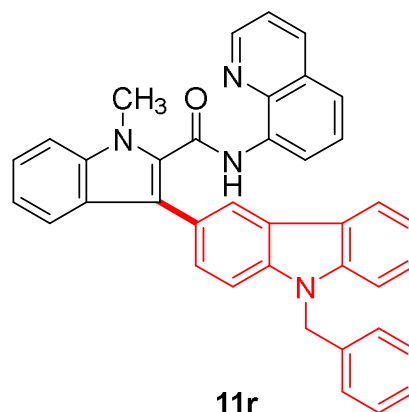
8.8500
8.8688

8.4233
8.4265

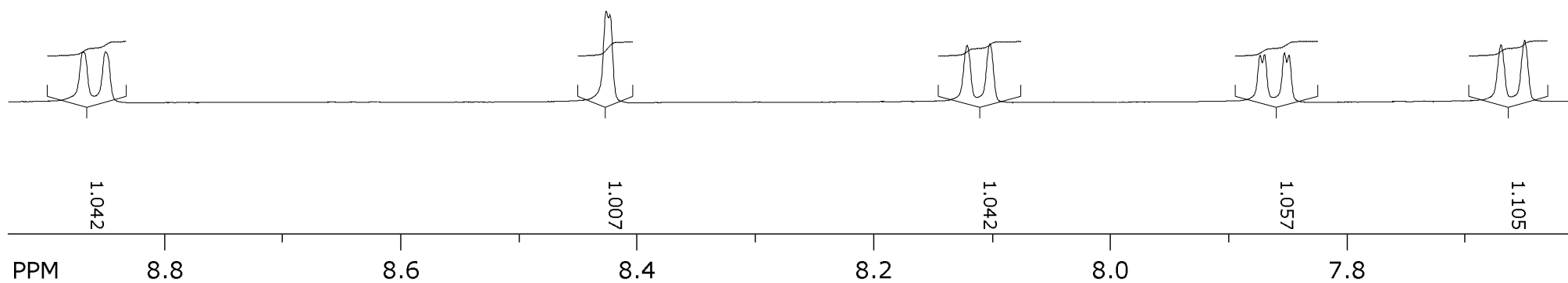
8.1017
8.1210

7.8487
7.8525
7.8694
7.8732

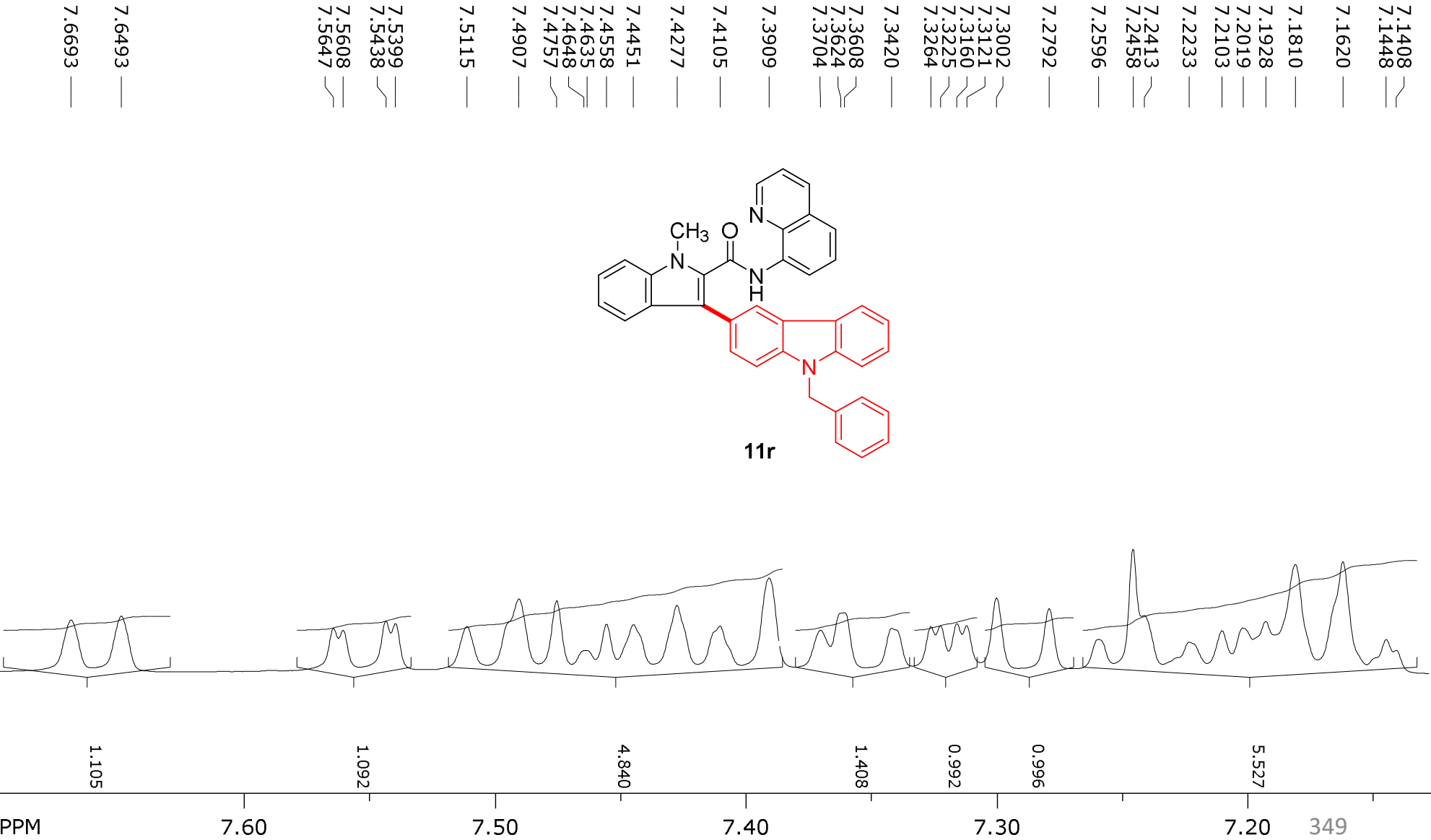
7.6493
7.6693



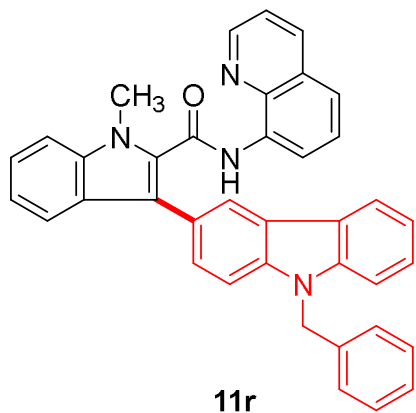
11r



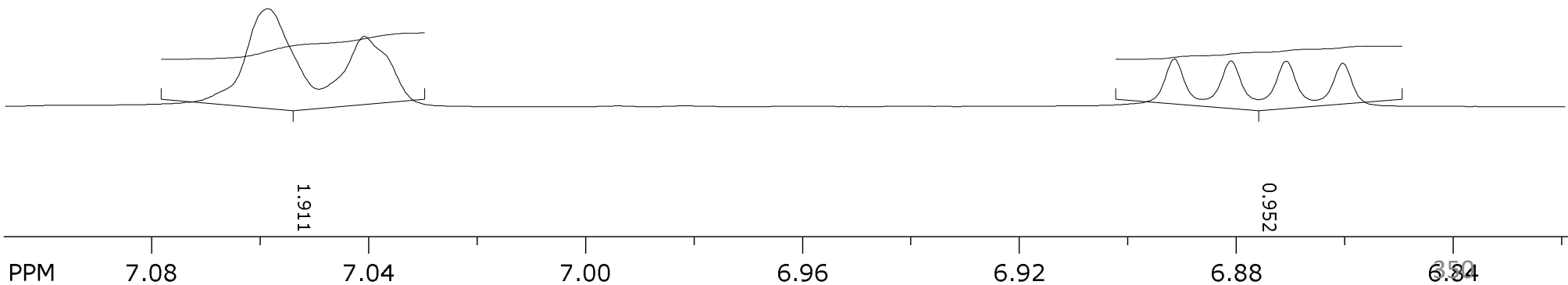
SpinWorks 4: RD 898
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: RD 898
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



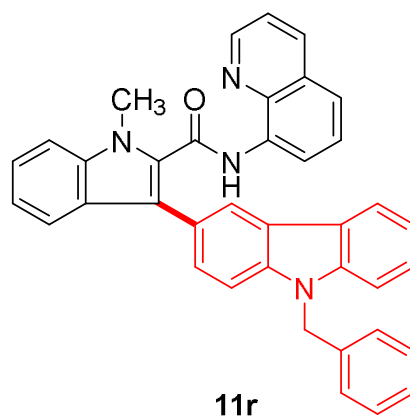
11r



SpinWorks 4: RD 898
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

5.4210

4.2320



11r

1.960

2.960

PPM

5.6

5.2

4.8

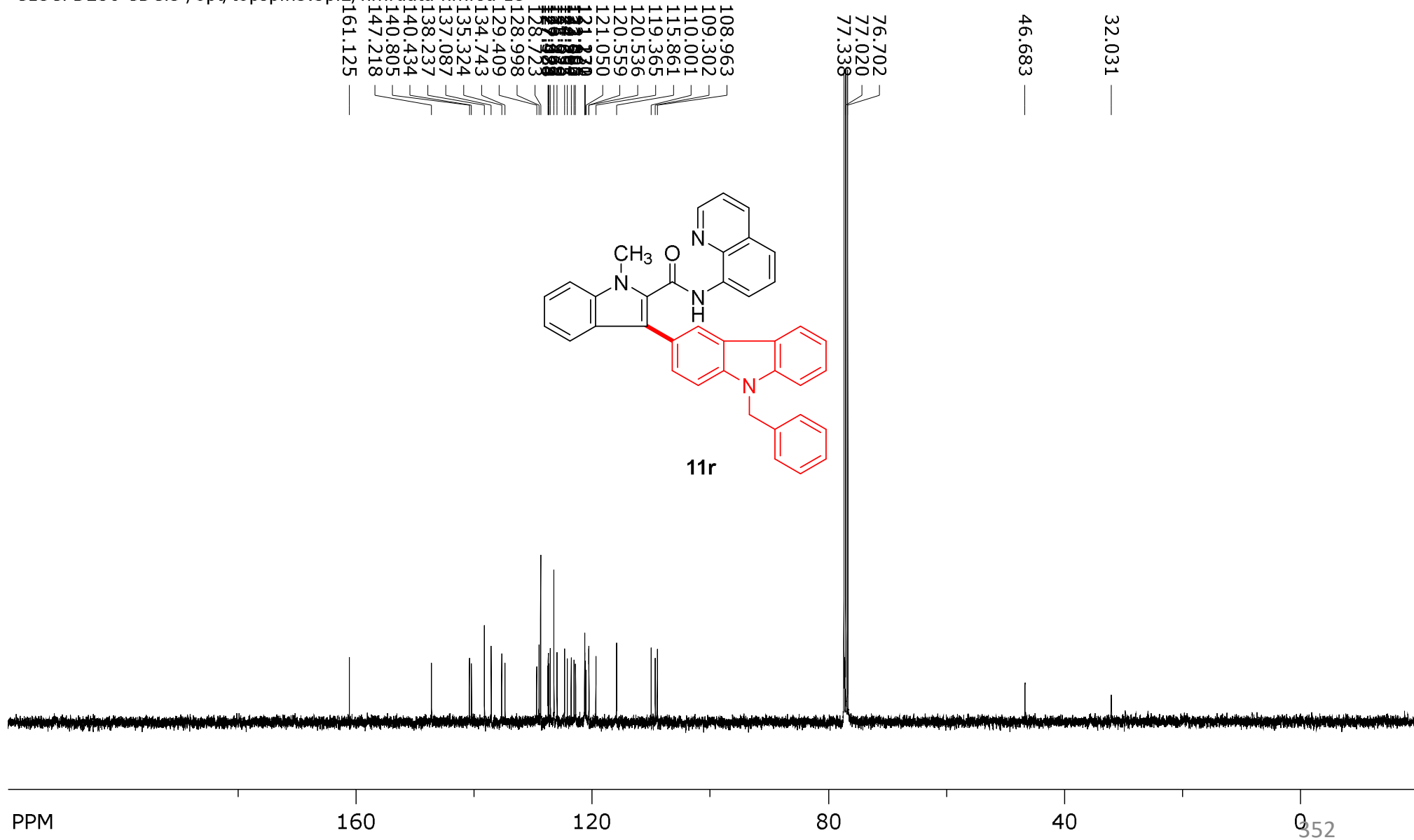
4.4

4.0

351

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 13

108.963
109.302
110.001
115.861
119.365
120.536
120.559
121.050
121.700
121.700
121.700
128.723
128.998
129.409
134.743
135.324
137.087
138.237
140.434
140.805
147.218
161.125



SpinWorks 4: RD-898

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 13

161.125 —

147.218 —

140.434 —
140.805 —

138.237 —
137.087 —

135.324 —
134.743 —

129.409 —

128.998 —

128.723 —

127.488 —

127.434 —

127.323 —

127.079 —

126.462 —

125.929 —

124.655 —

124.202 —

123.554 —

123.080 —

122.805 —

121.272 —

121.231 —

121.170 —

120.559 —

120.536 —

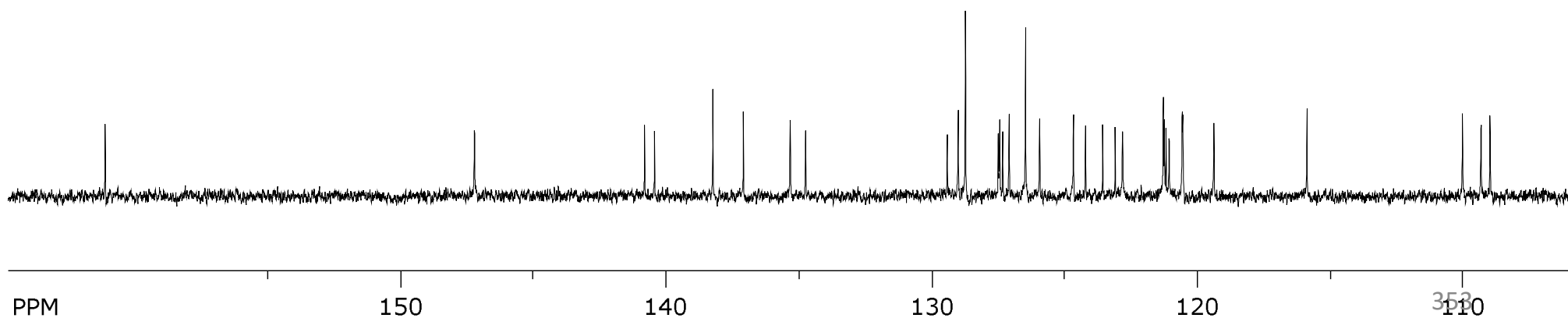
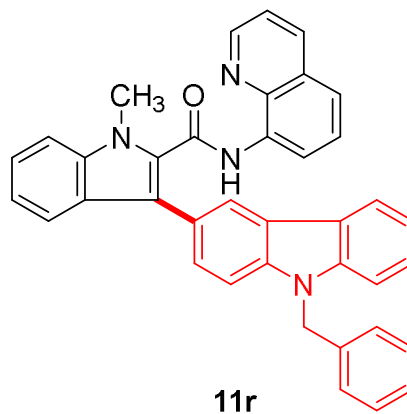
119.365 —

115.861 —

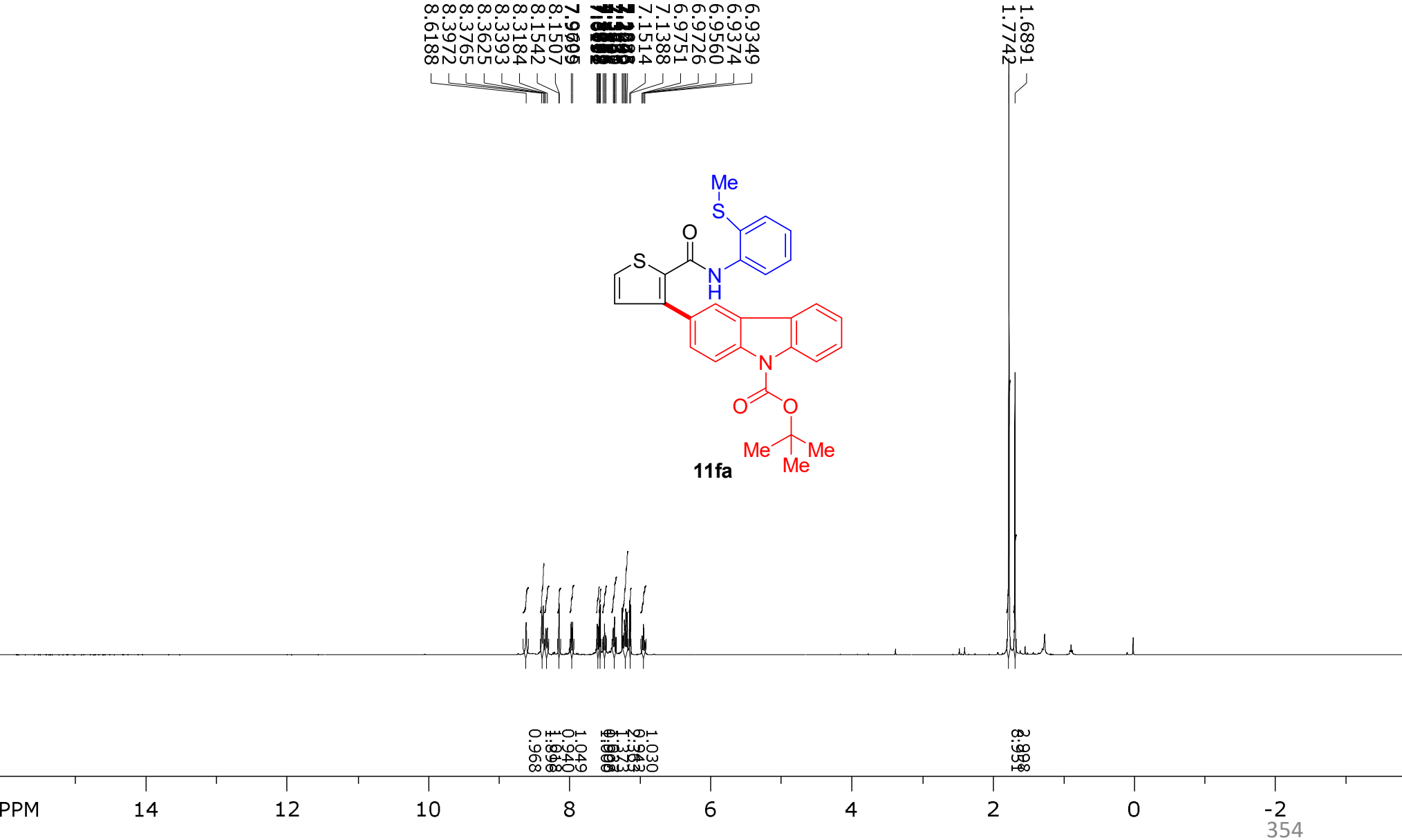
110.001 —

109.302 —

108.963 —



SpinWorks 4: RD 457
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23



SpinWorks 4: RD 457
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23

8.6188

8.3972

8.3765

8.3625

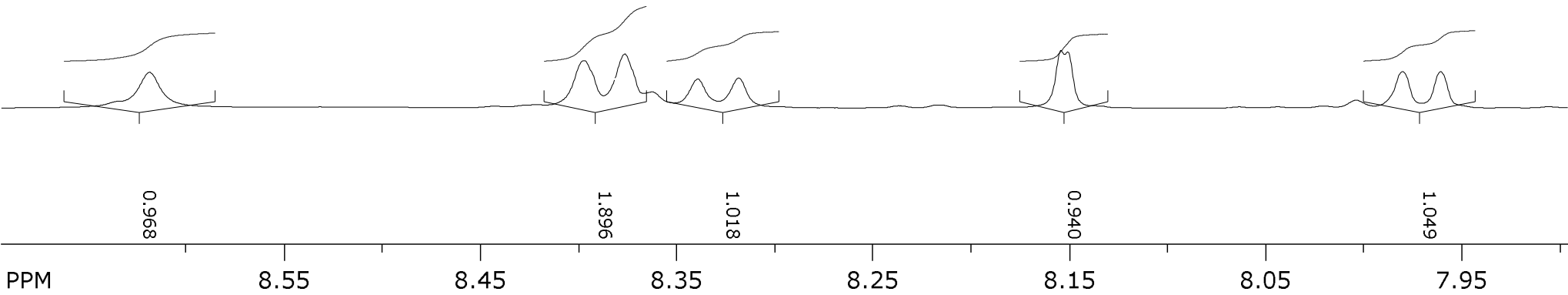
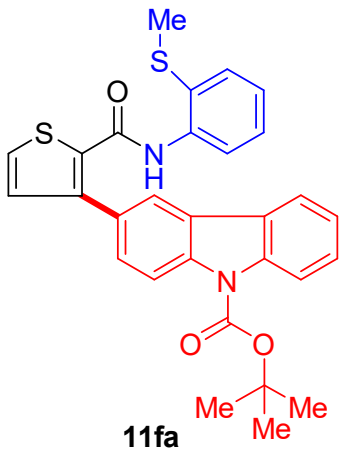
8.3393

8.3184

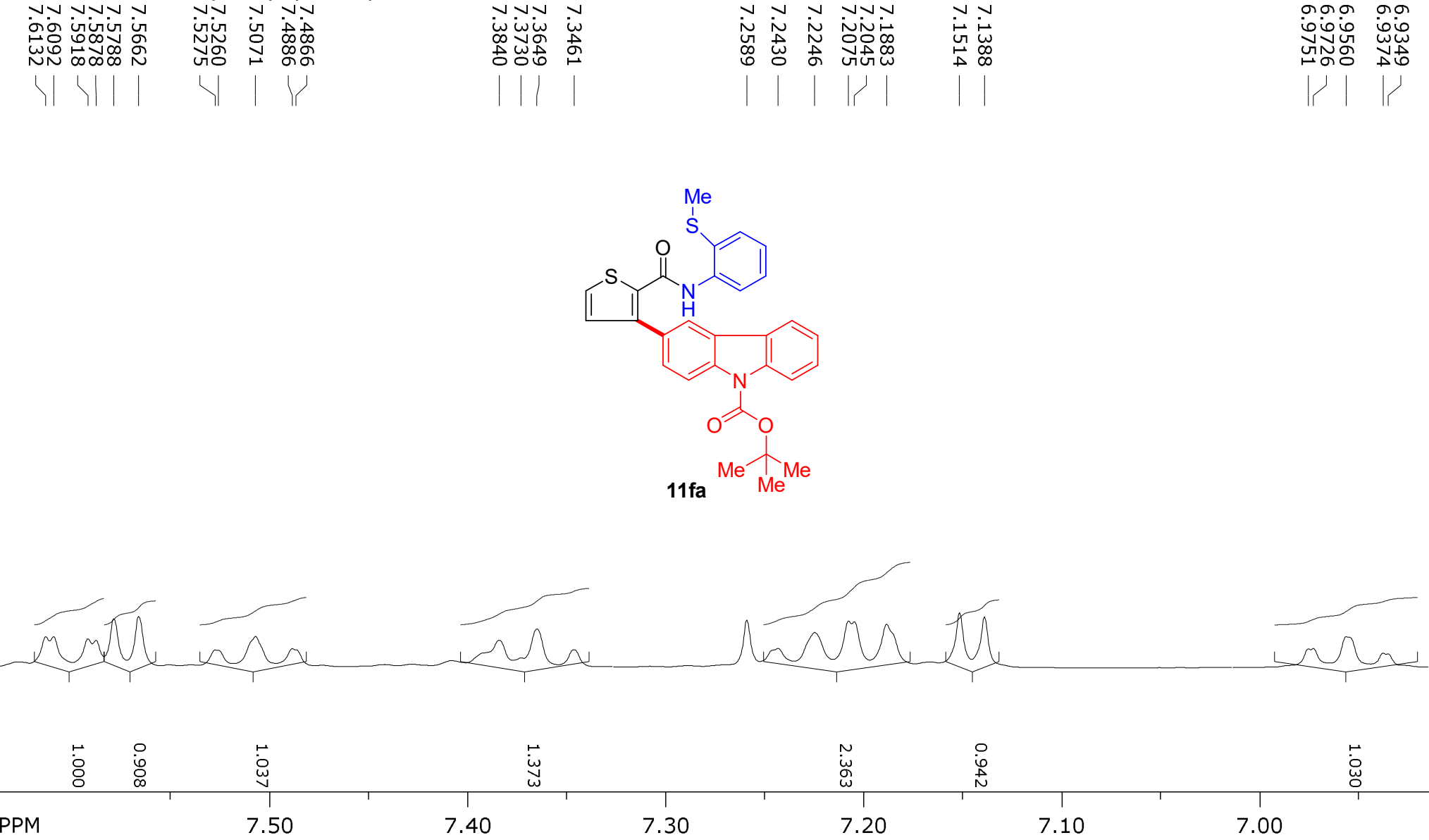
8.1507
8.1542

7.9799

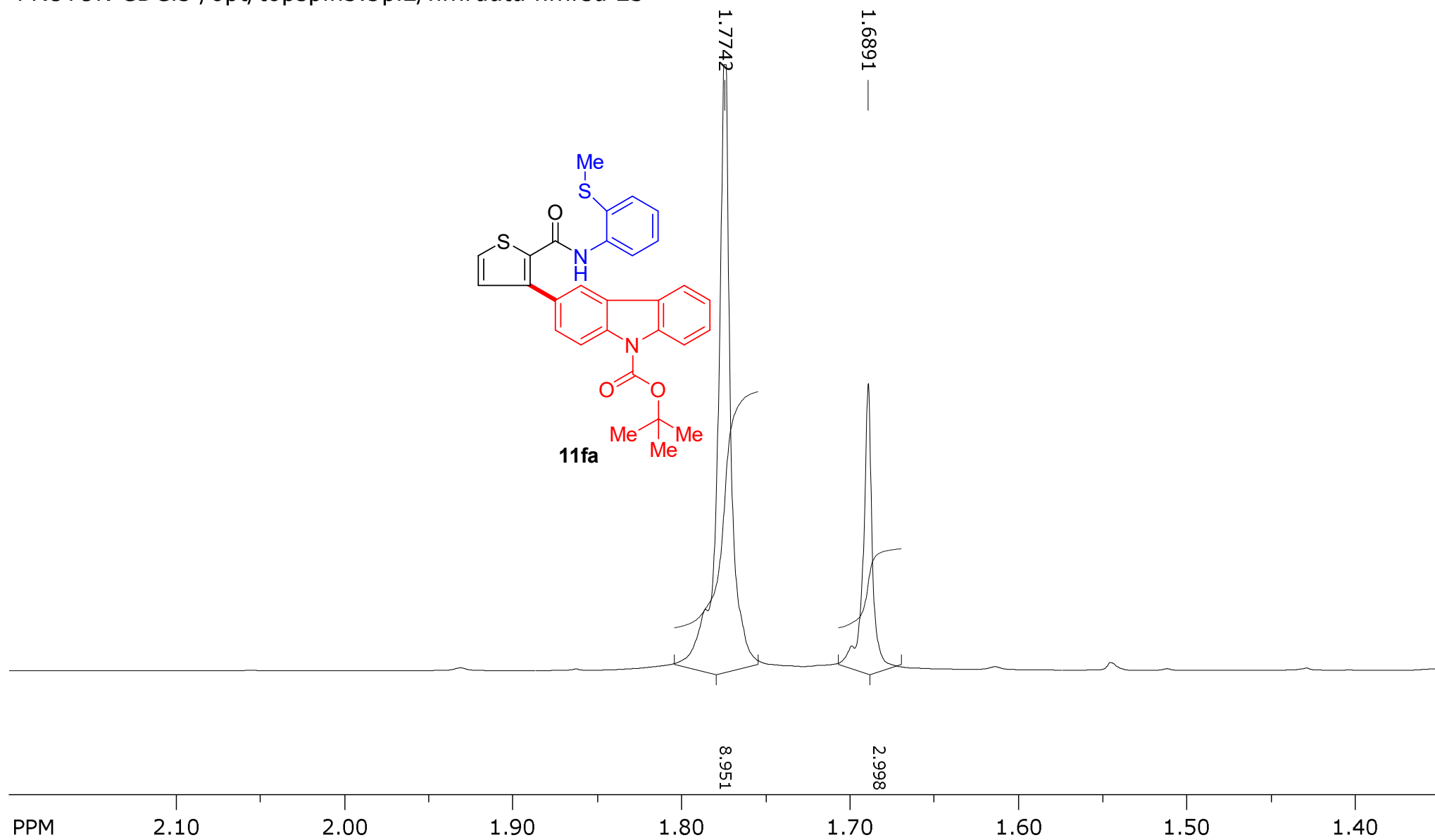
7.9605



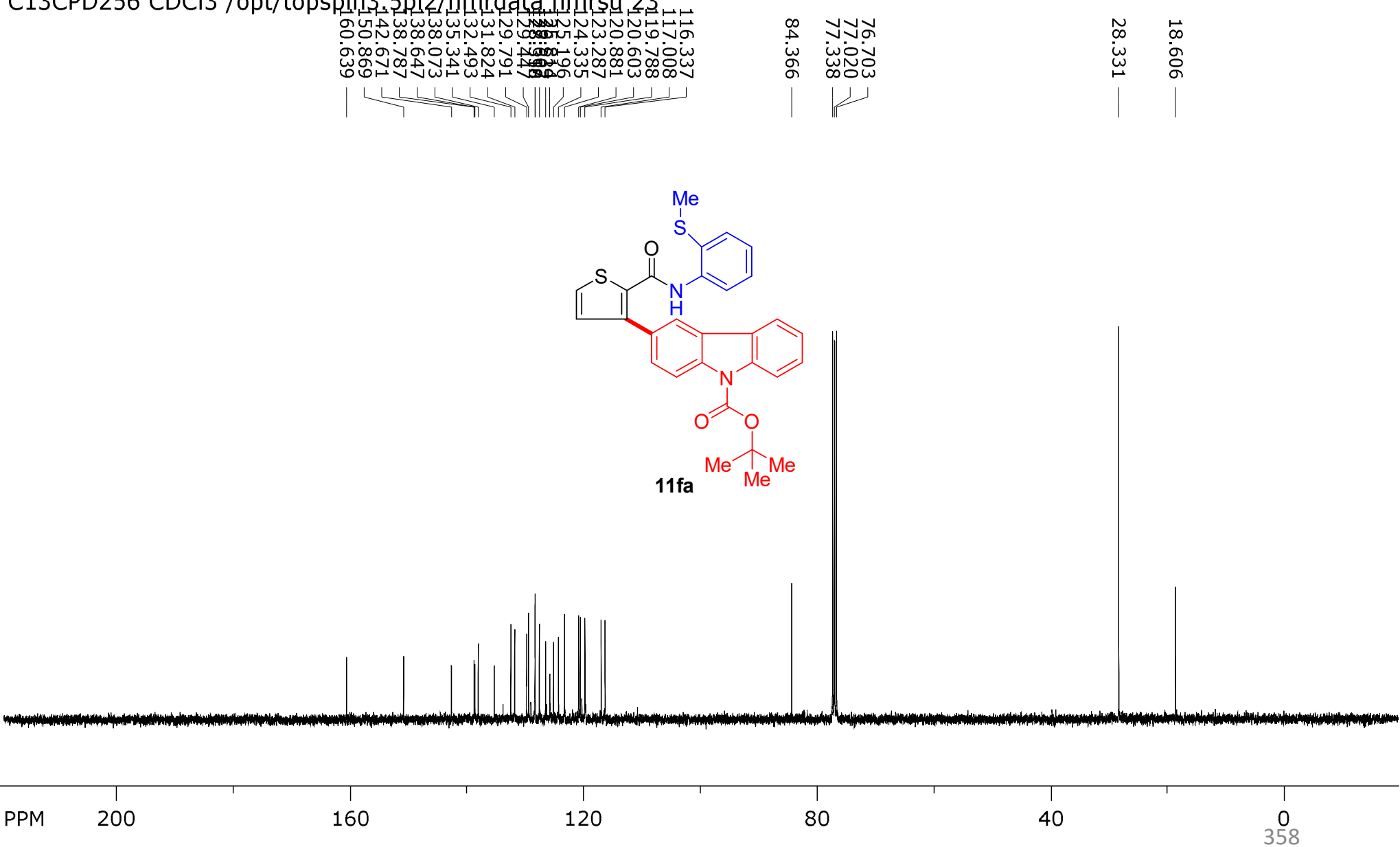
SpinWorks 4: RD 457
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23



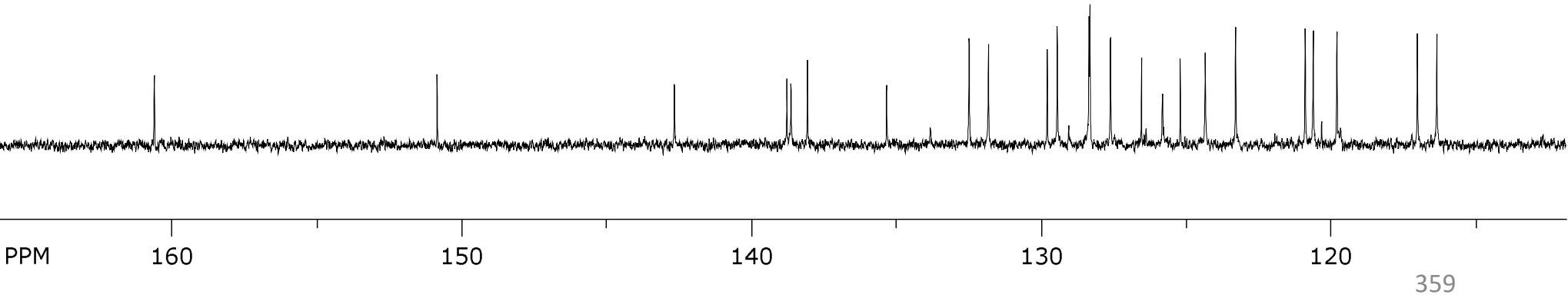
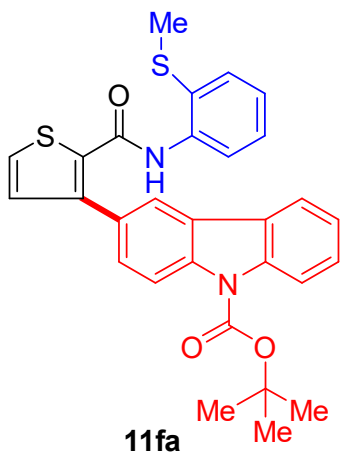
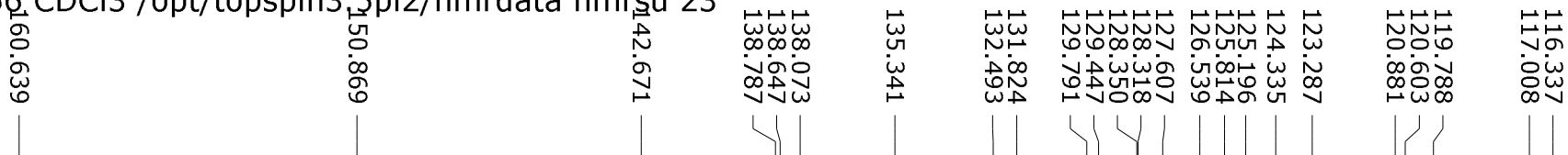
SpinWorks 4: RD 457
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23



SpinWorks 4: RD 457
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata/nmr su 23



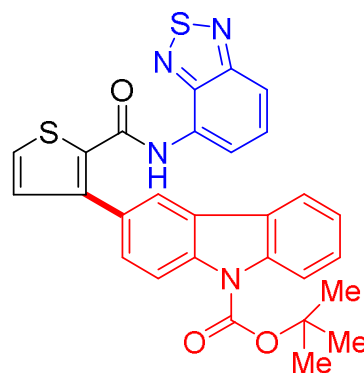
SpinWorks 4: RD 457
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23



SpinWorks 4: RD-524

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

7.2152
7.2278
7.2597
7.3303
7.3318
7.3500
7.3677
7.3693
7.3709
7.9284
8.2037
8.3804
8.4119
8.4288
8.4332
8.4366
8.4410
8.4495
8.9285



11fb

1.245
1.017
1.016
3.209
0.977

1.7847

9.000

PPM

12

8

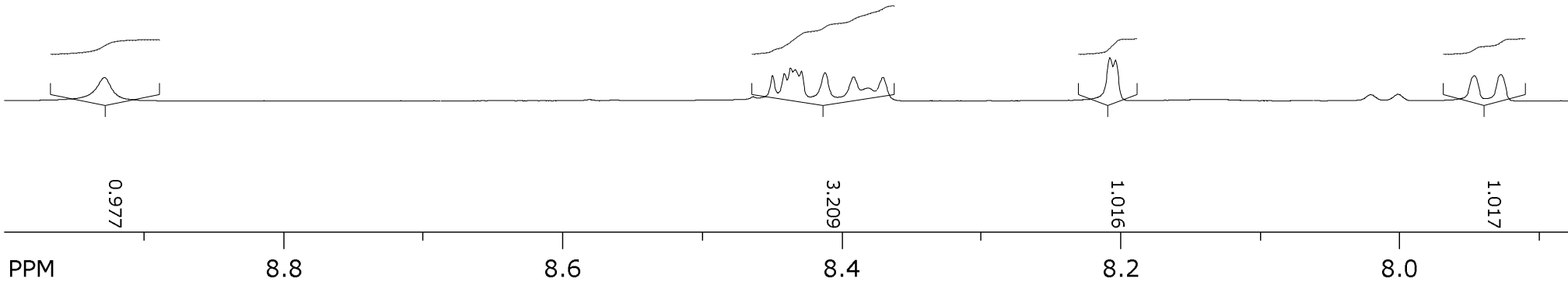
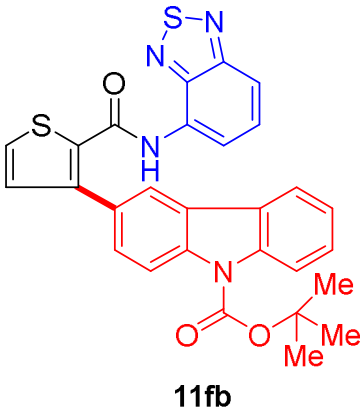
4

0

360

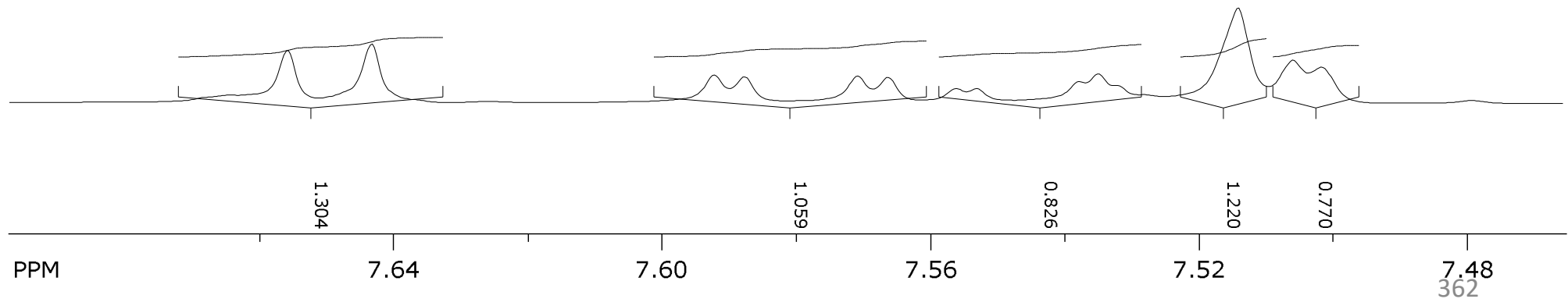
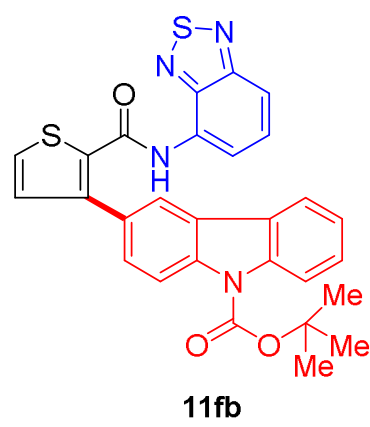
SpinWorks 4: RD-524
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

8.9285 —
8.3704 —
8.3812 —
8.3914 —
8.4119 —
8.4288 —
8.4332 —
8.4366 —
8.4410 —
8.4495 —
8.2037 —
8.2077 —
7.9274 —
7.9464 —



SpinWorks 4: RD-524
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

7.6559	7.6434	7.5923	7.5877	7.5709	7.5663	7.5531	7.5562	7.5378	7.5350	7.5322	7.5282	7.5141	7.5060	7.5017
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



SpinWorks 4: RD-524

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

7.3677
7.3693

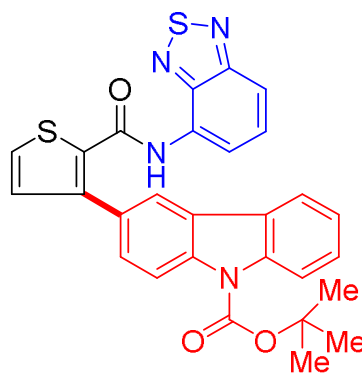
7.3500

7.3303
7.3318

7.2597

7.2278

7.2152



11fb

1.055

1.246

PPM

7.36

7.32

7.28

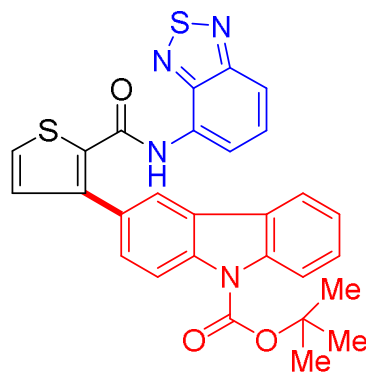
7.24

7.20

363

SpinWorks 4: RD-524 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

114.826
115.576
116.421
117.570
119.981
120.421
123.333
125.354
127.145
127.957
129.736
130.231
130.931
131.717
135.088
138.891
138.946
143.459
147.343
150.946
154.348
160.578
84.466
77.703
77.020
77.338
28.393



11fb



PPM

160

120

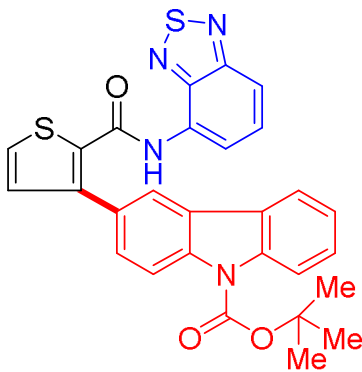
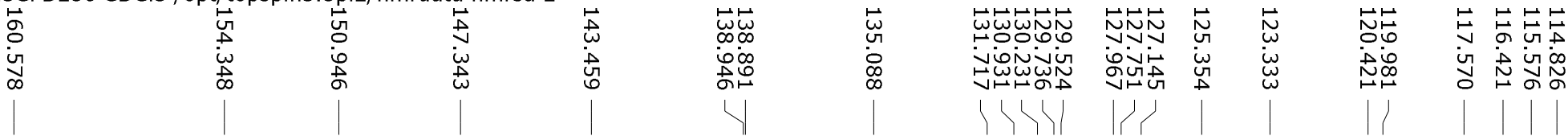
80

40

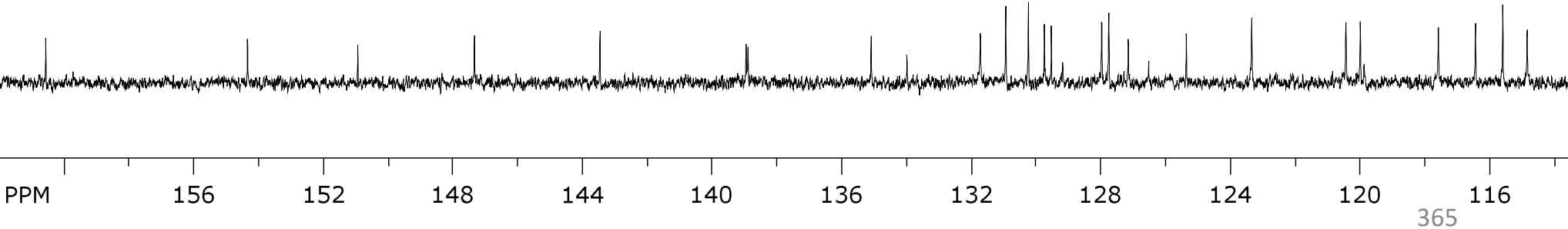
0

364

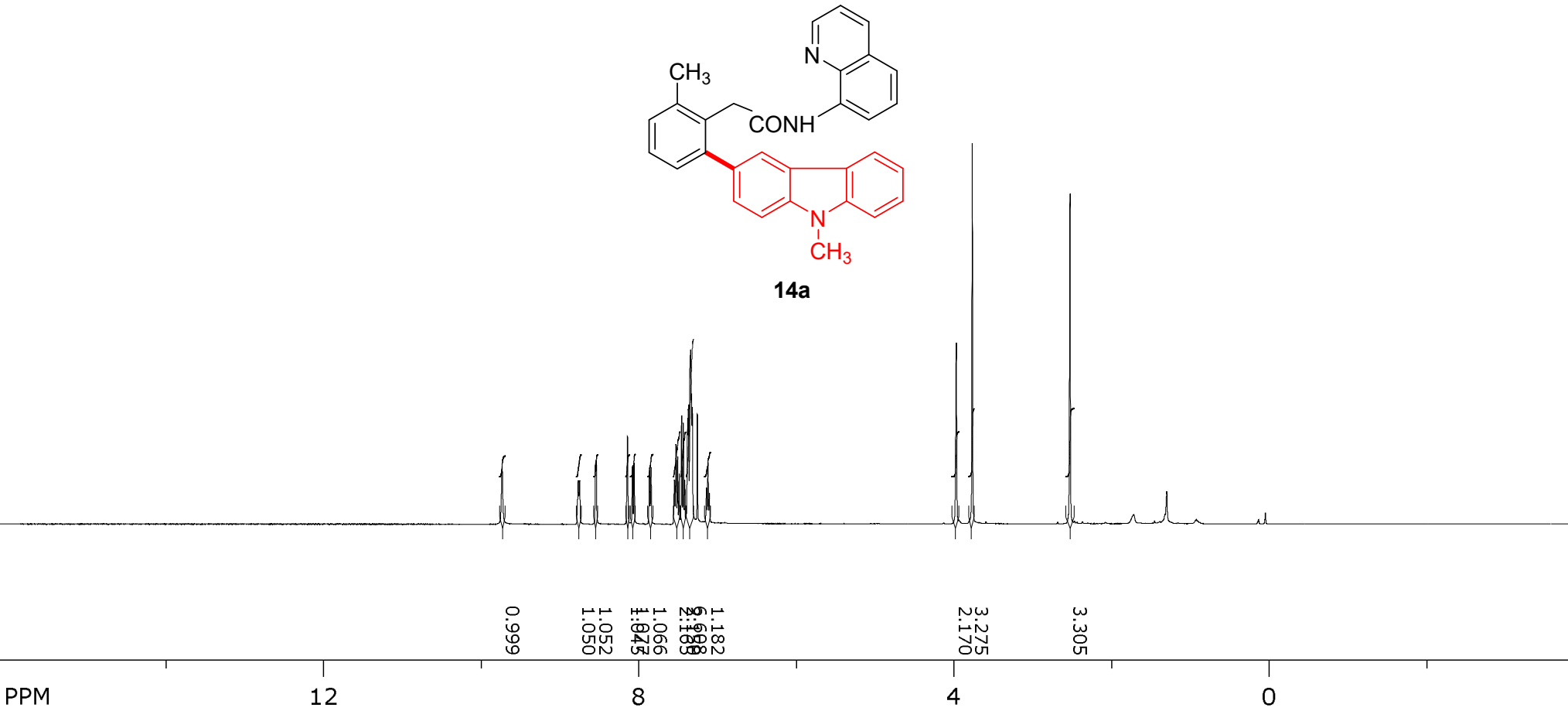
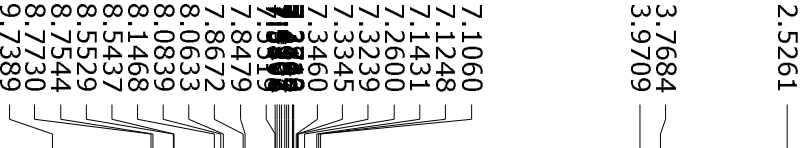
SpinWorks 4: RD-524 RE
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



11fb



SpinWorks 4: RD 491
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



SpinWorks 4: RD 491

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

9.7389

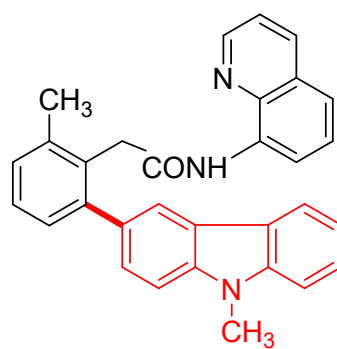
8.7544
8.7730

8.5437
8.5529

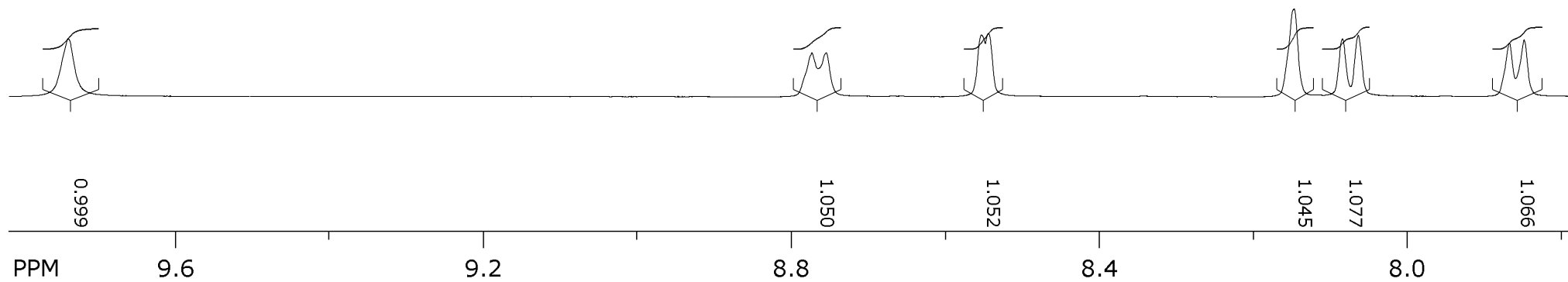
8.1468

8.0633
8.0839

7.8479
7.8672

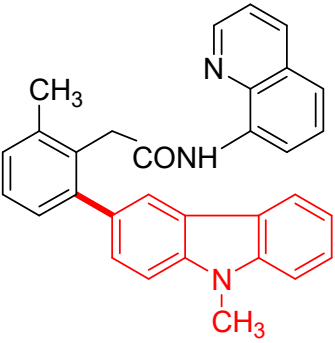


14a

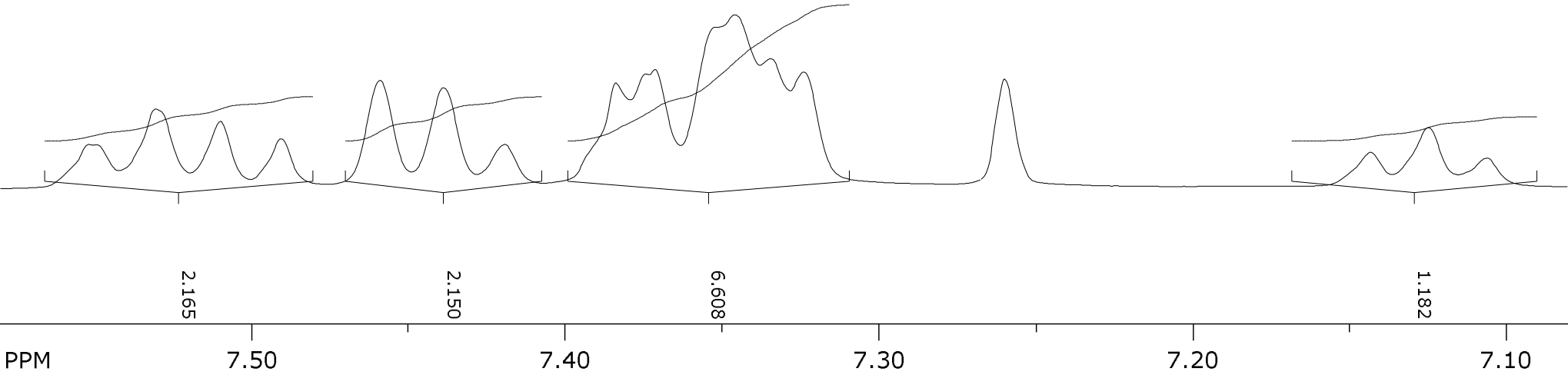


SpinWorks 4: RD 491
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

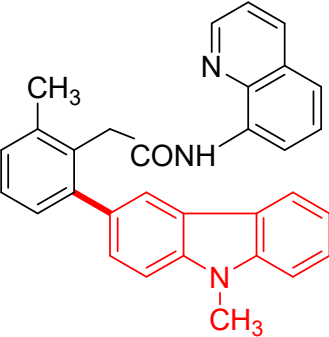
7.5519
7.5494
7.5306
7.5101
7.4907
7.4592
7.4389
7.4194
7.3839
7.3743
7.3713
7.3460
7.3345
7.3239
7.2600
7.1431
7.1248
7.1060



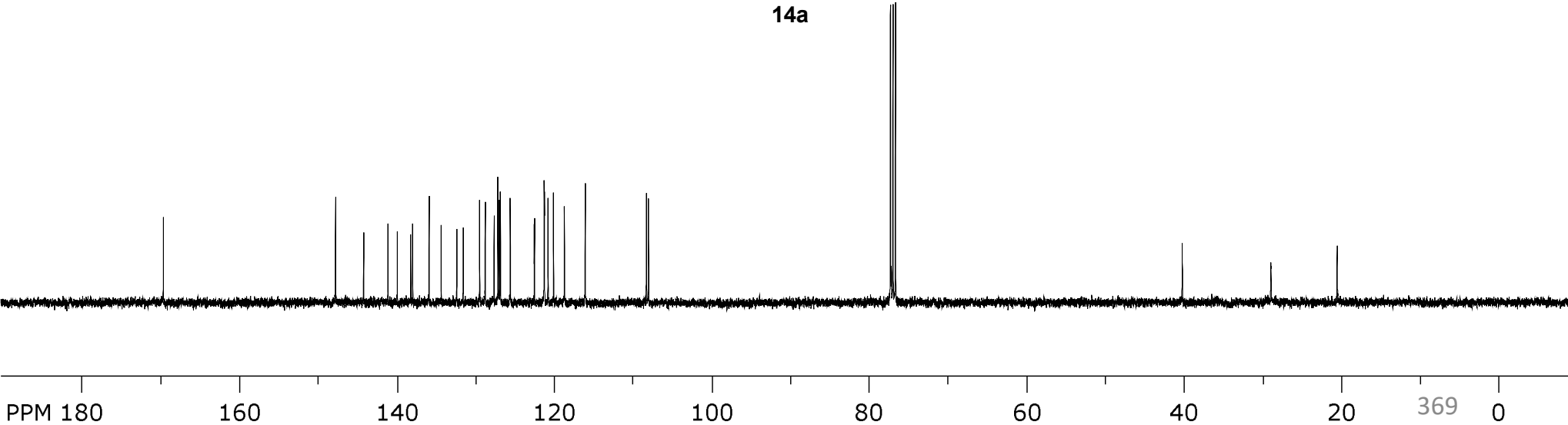
14a



SpinWorks 4: RD 491
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

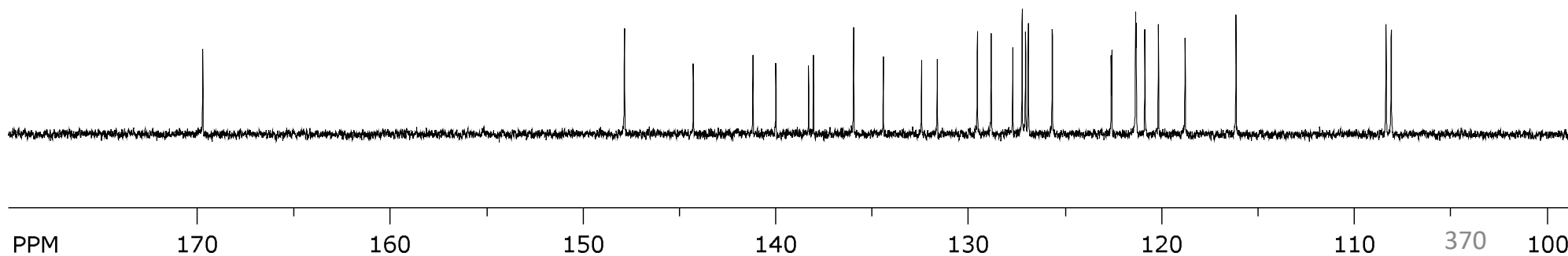
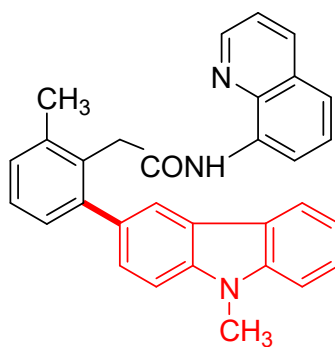


14a



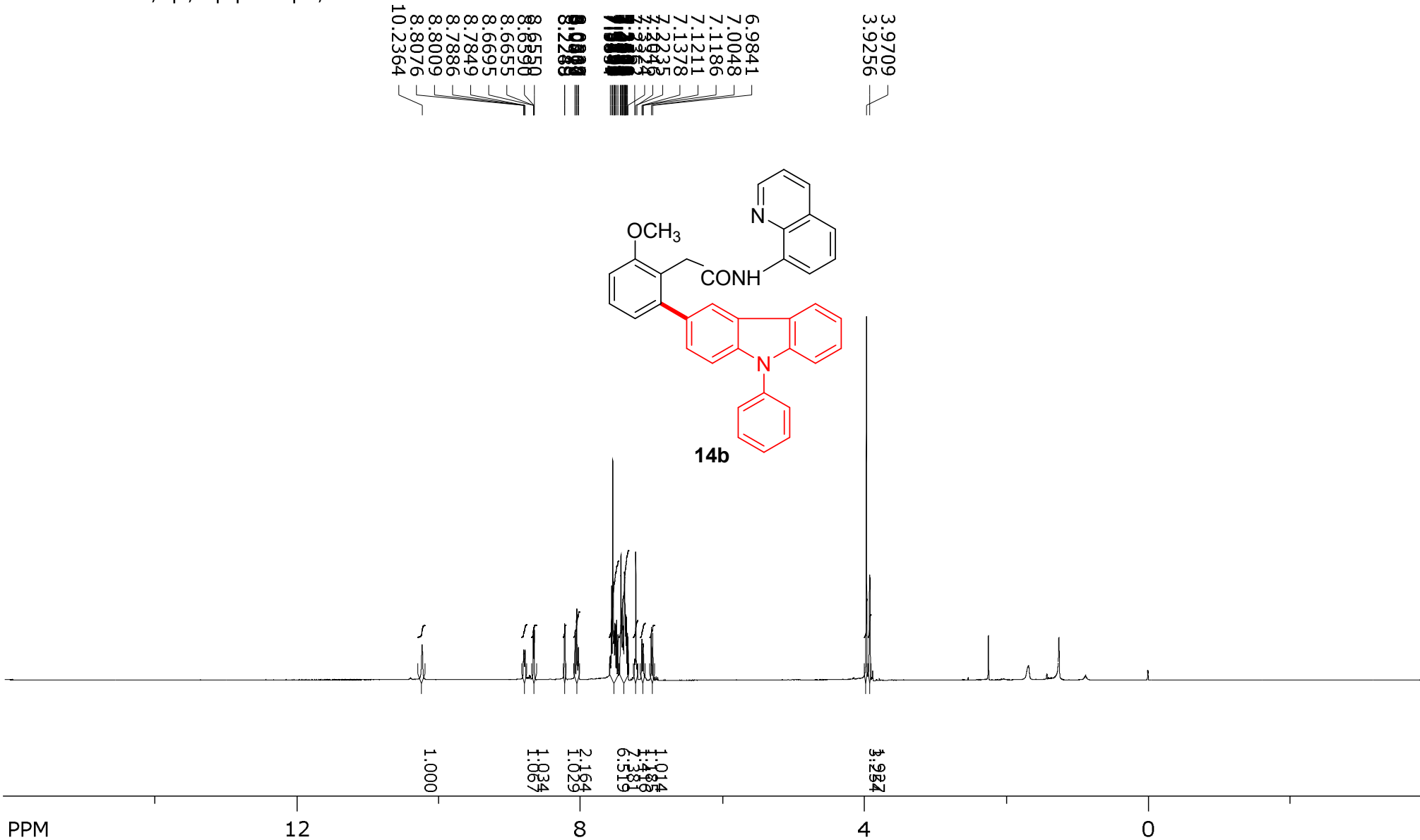
SpinWorks 4: RD 491
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

169.741 —
147.856 —
144.285 —
141.188 —
139.998 —
138.051 —
138.299 —
135.962 —
134.422 —
132.442 —
131.627 —
129.544 —
128.823 —
127.706 —
127.219 —
127.042 —
126.899 —
125.654 —
122.594 —
122.566 —
121.328 —
121.300 —
120.850 —
120.148 —
118.762 —
116.121 —
108.334 —
108.065 —



SpinWorks 4: RD-1240

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

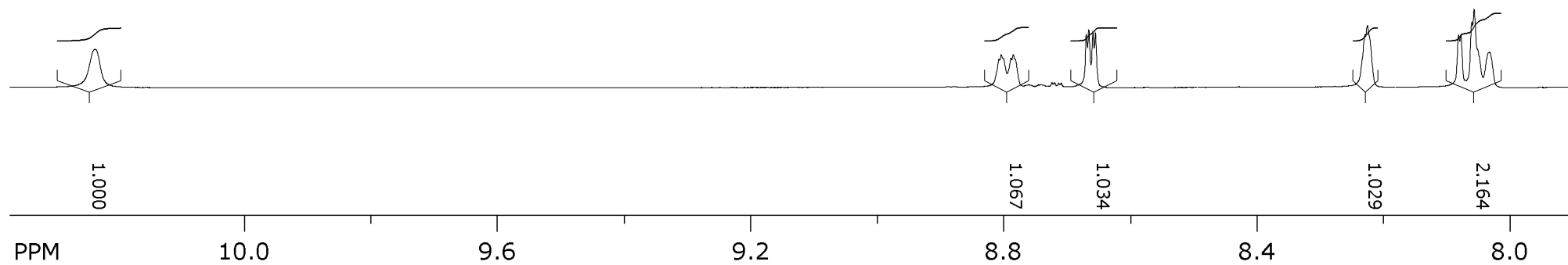
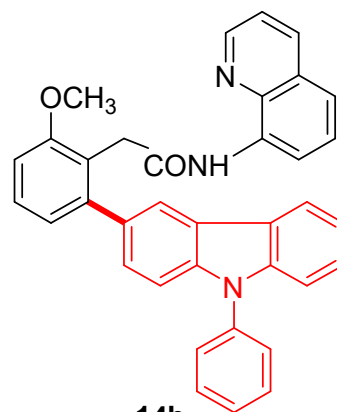


SpinWorks 4: RD-1240
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

10.2364

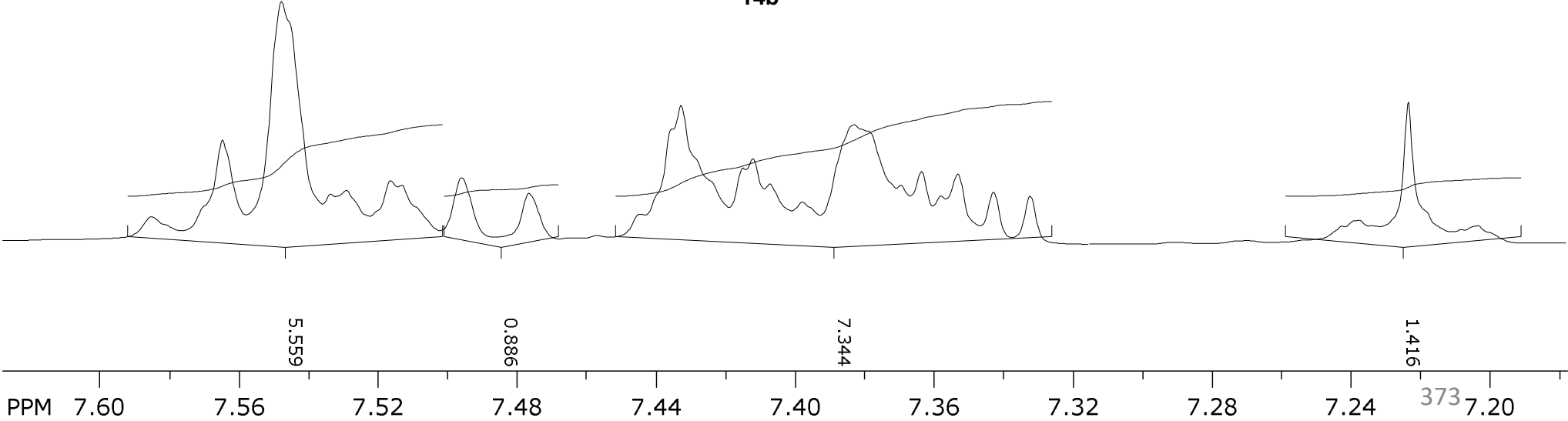
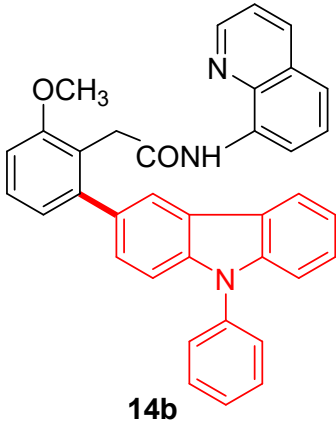
8.6550
8.6590
8.6655
8.6695
8.7849
8.7886
8.8009
8.8076

8.0317
8.0339
8.0564
8.0600
8.0773
8.0810
8.2249
8.2288



SpinWorks 4: RD-1240
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

7.5854 —
7.5649 —
7.5479 —
7.5292 —
7.5338 —
7.5166 —
7.5132 —
7.4960 —
7.4766 —
7.4449 —
7.4354 —
7.4329 —
7.4151 —
7.4122 —
7.4073 —
7.3979 —
7.3829 —
7.3808 —
7.3790 —
7.3695 —
7.3636 —
7.3580 —
7.3532 —
7.3429 —
7.3324 —
7.2362 —
7.2235 —
7.2046 —



SpinWorks 4: RD-1240

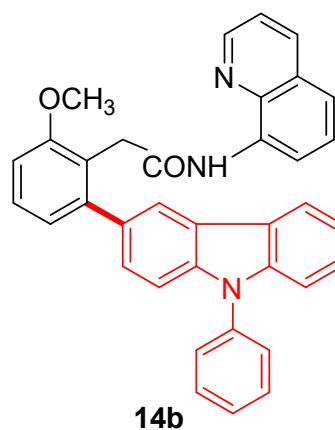
PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 40

7.1378

7.1186
7.1211

7.0048

6.9841



1.185

1.014

PPM

7.16

7.12

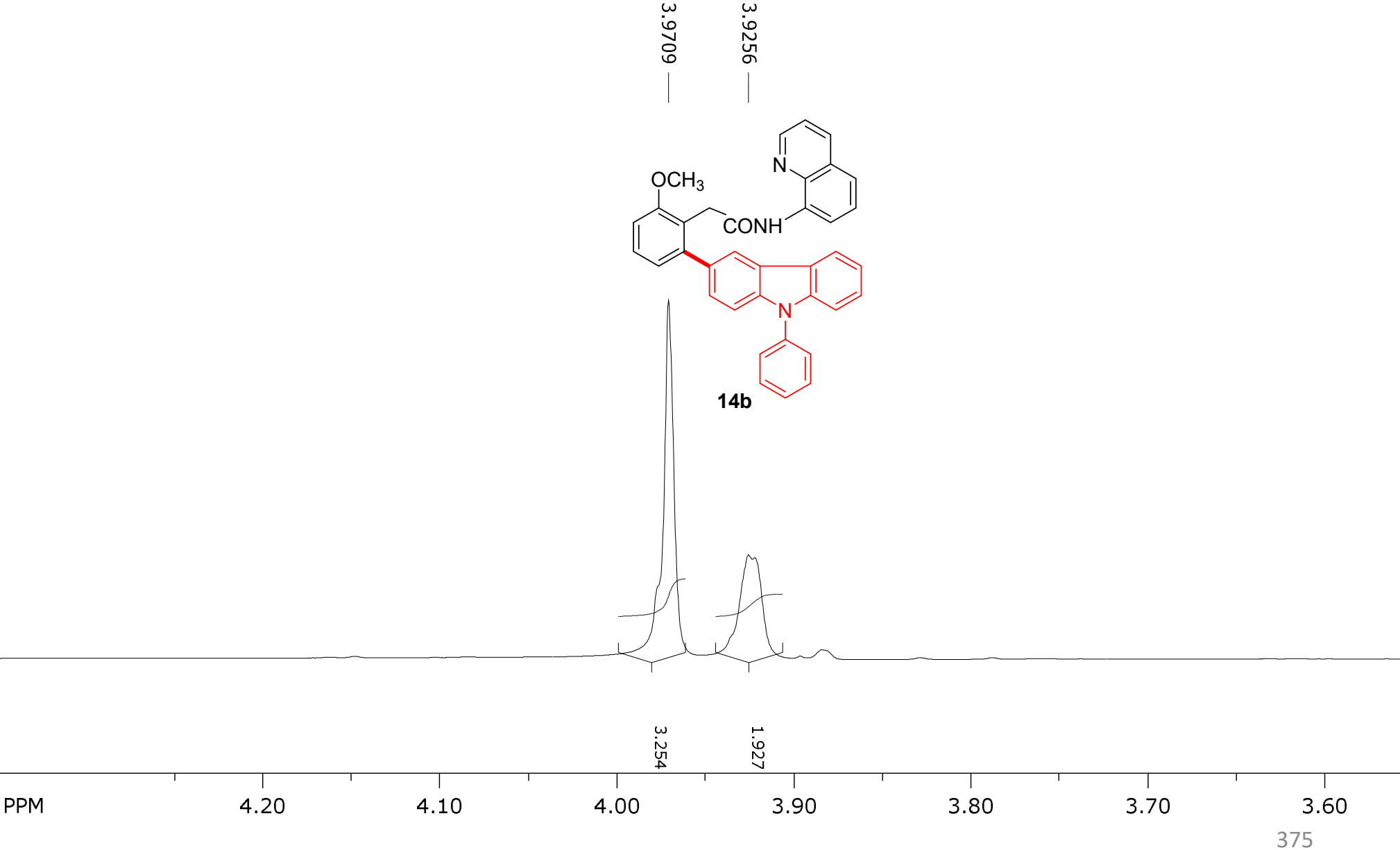
7.08

7.04

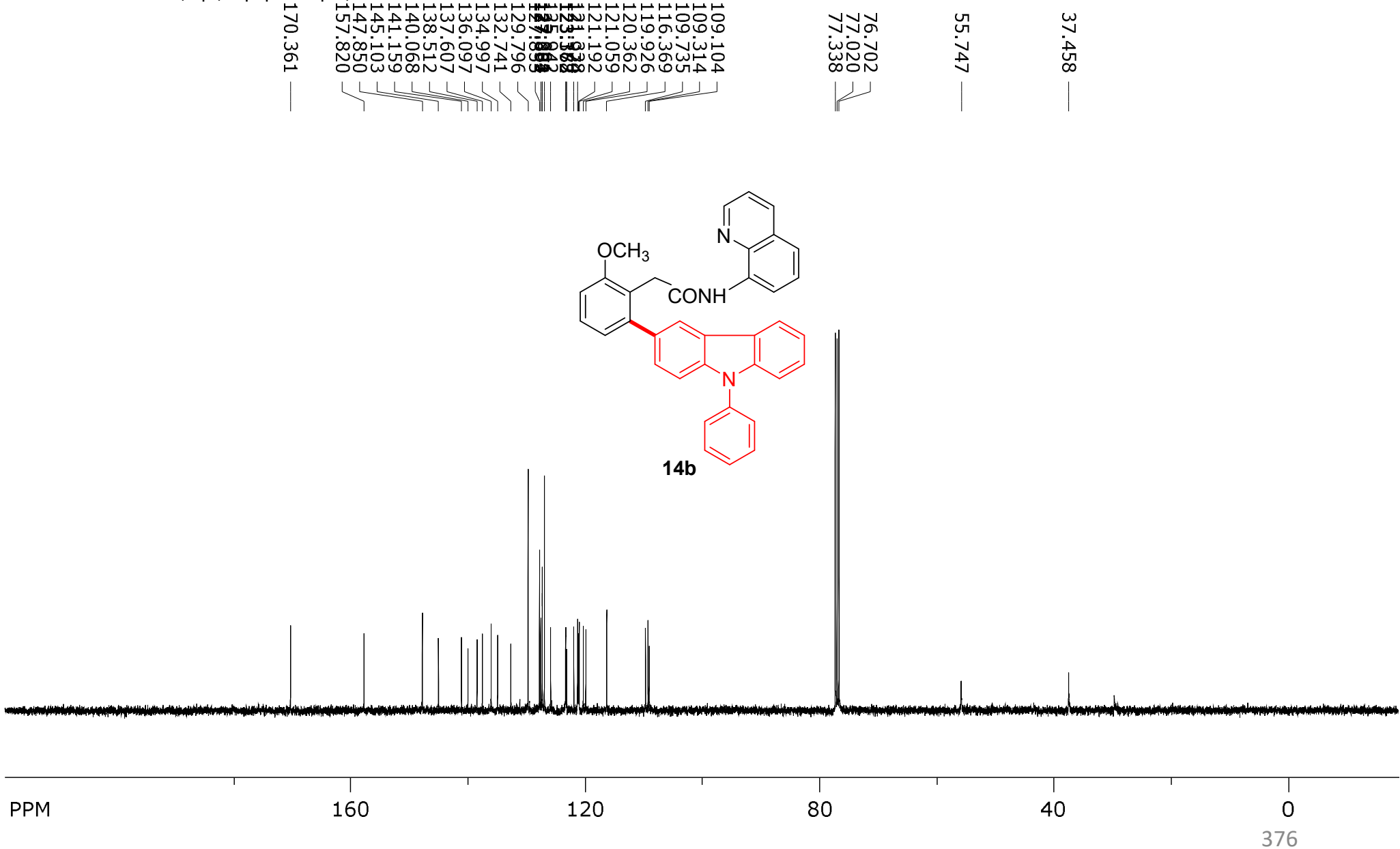
7.00

6.96

SpinWorks 4: RD-1240
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

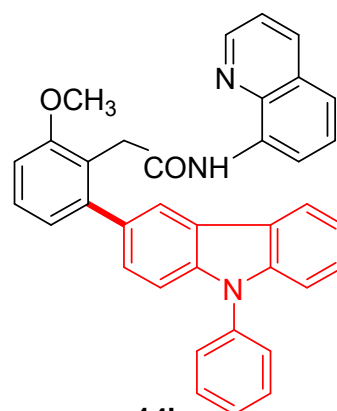


SpinWorks 4: RD-1240
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

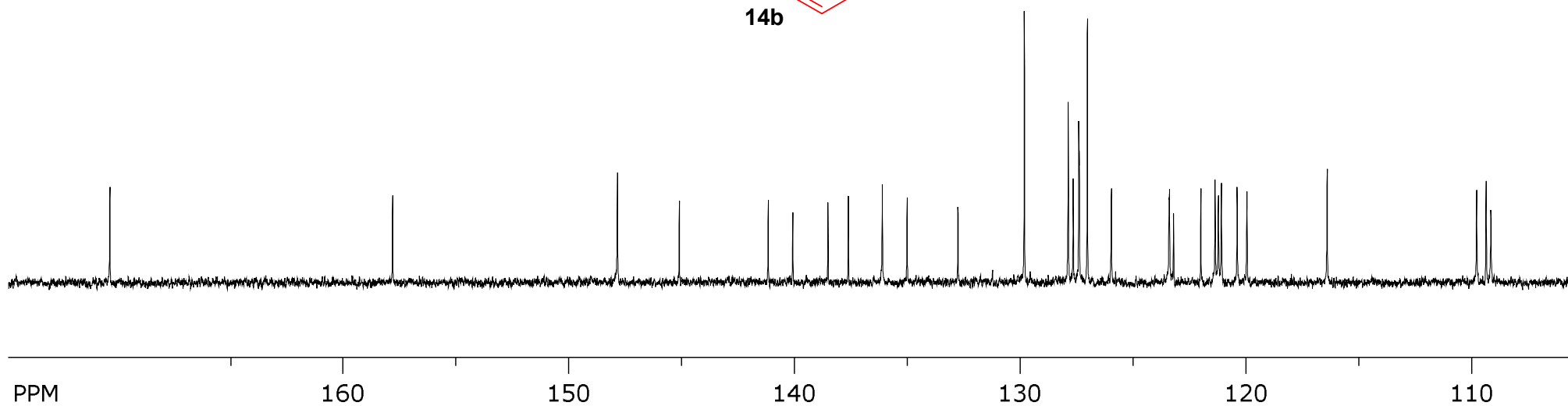


SpinWorks 4: RD-1240
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

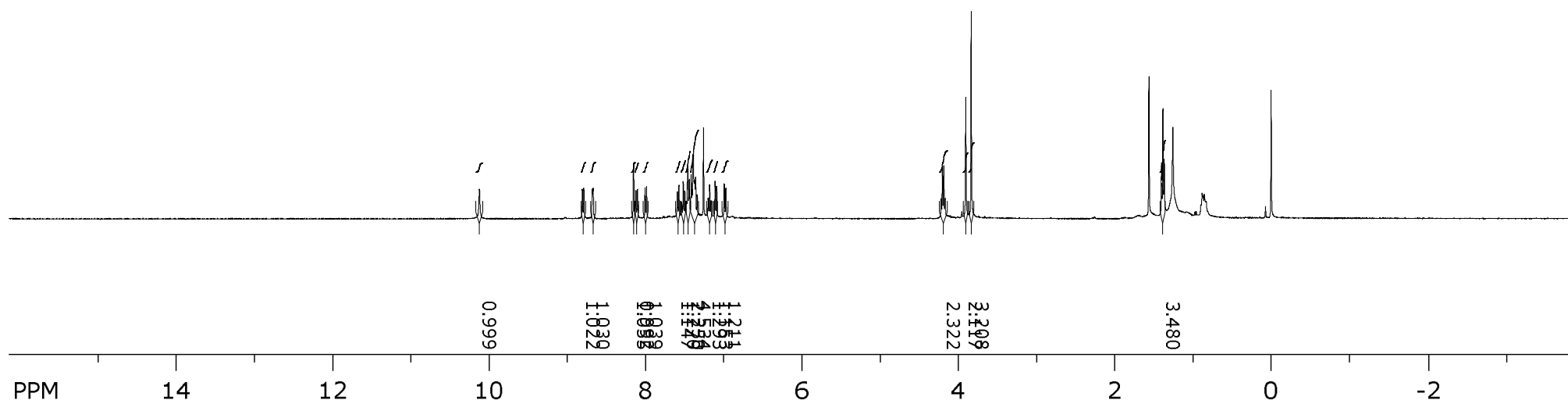
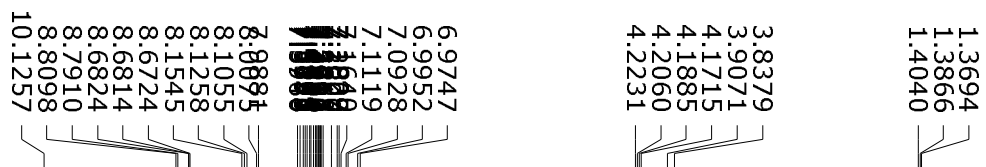
170.361 —
157.820 —
147.850 —
145.103 —
141.159 —
140.068 —
138.512 —
137.607 —
136.097 —
134.997 —
132.741 —
129.796 —
127.853 —
127.632 —
127.383 —
127.364 —
127.001 —
125.942 —
123.378 —
123.362 —
123.183 —
121.974 —
121.338 —
121.192 —
121.059 —
120.362 —
119.926 —
116.369 —
109.104 —
109.314 —
109.735 —



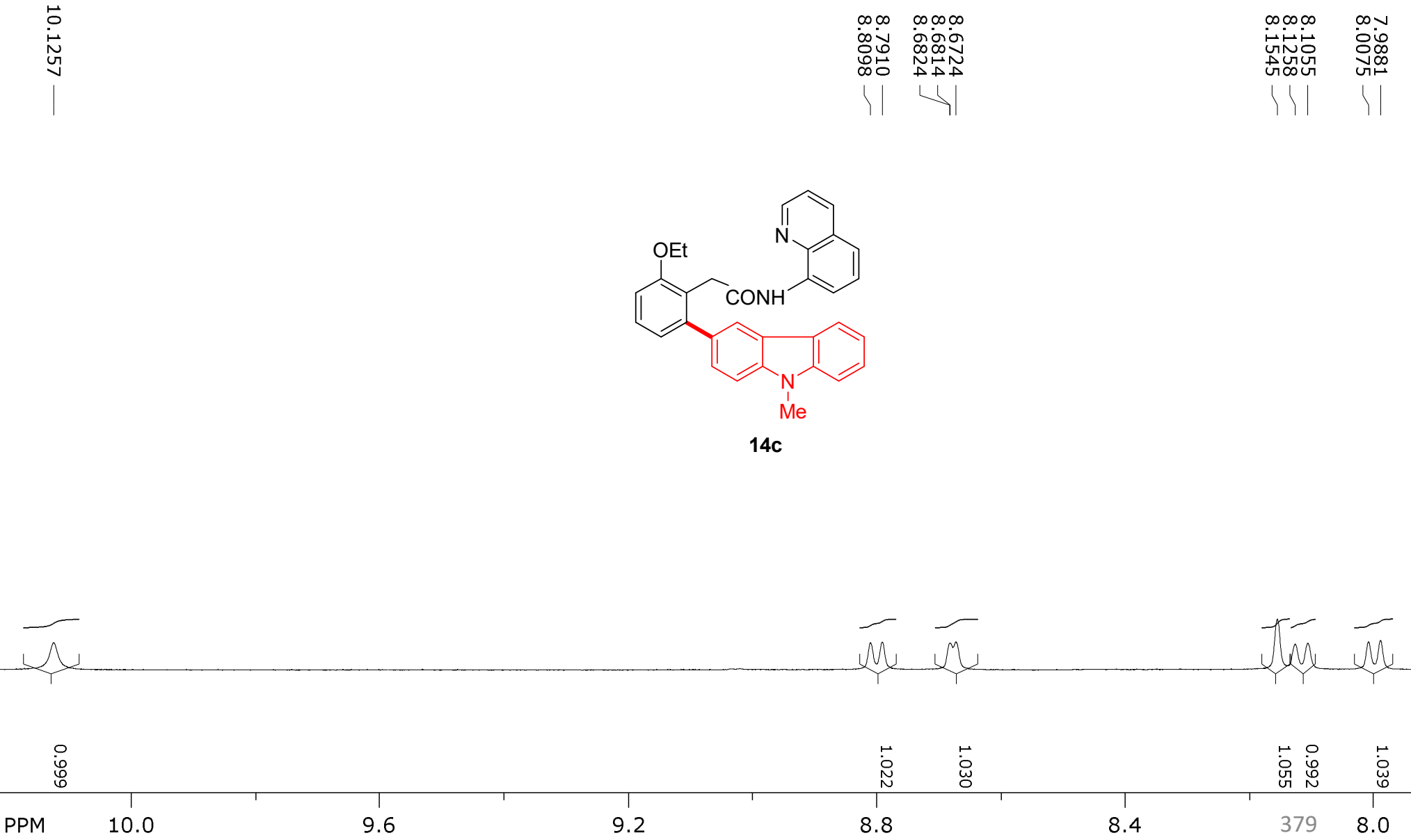
14b

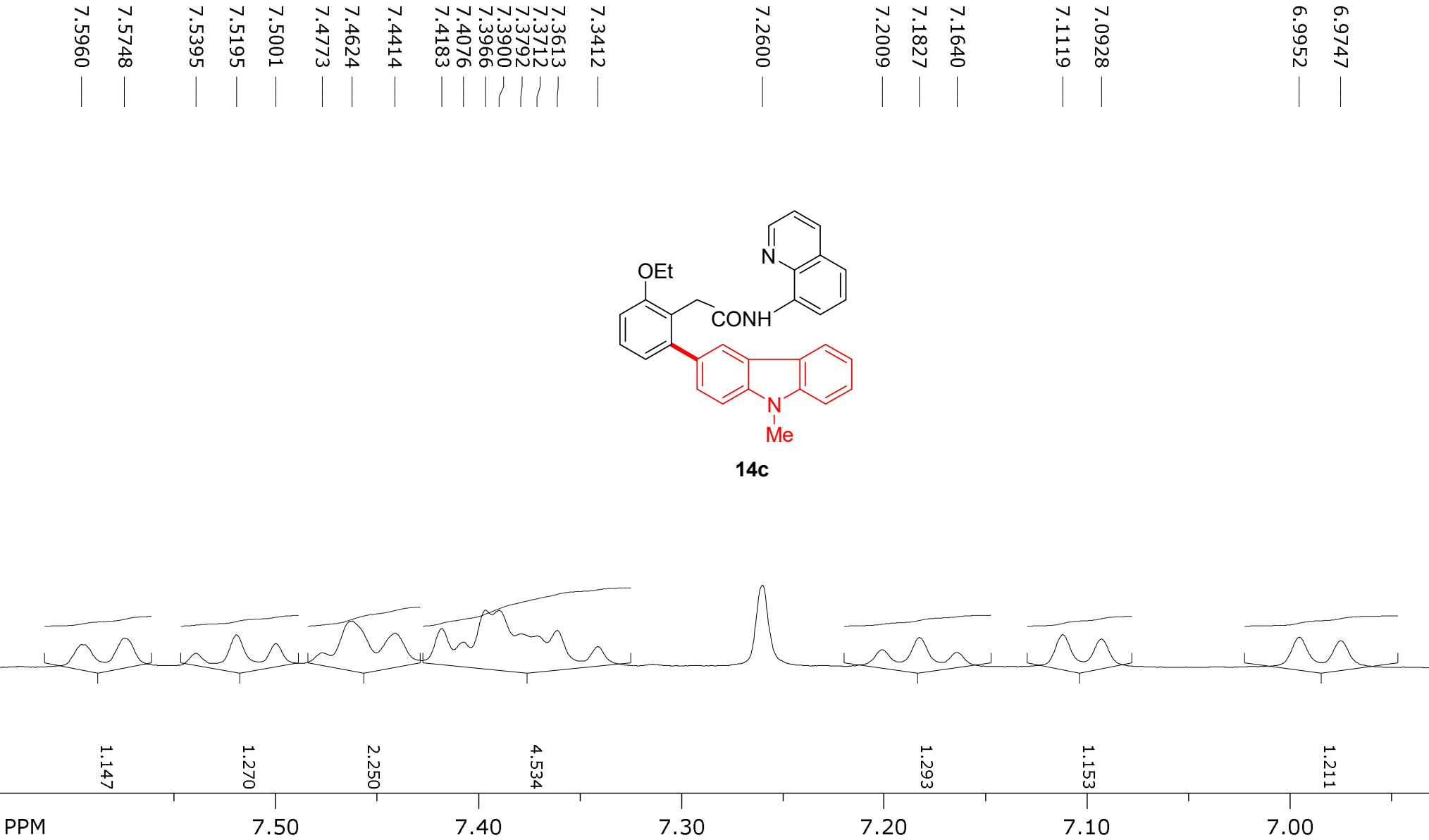


SpinWorks 4: RD 726

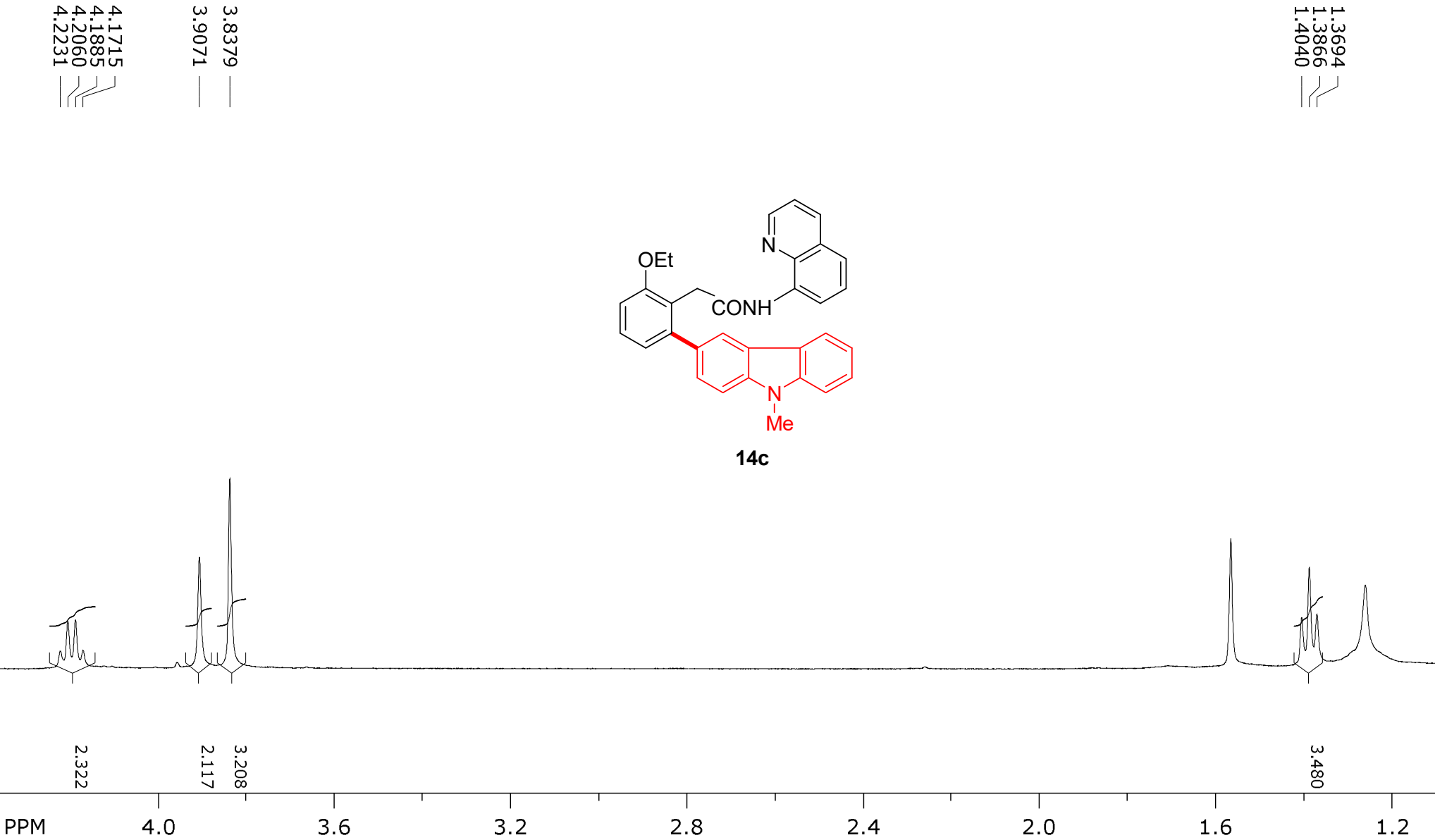


SpinWorks 4: RD 726



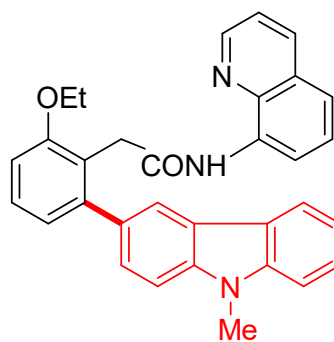


SpinWorks 4: RD 726

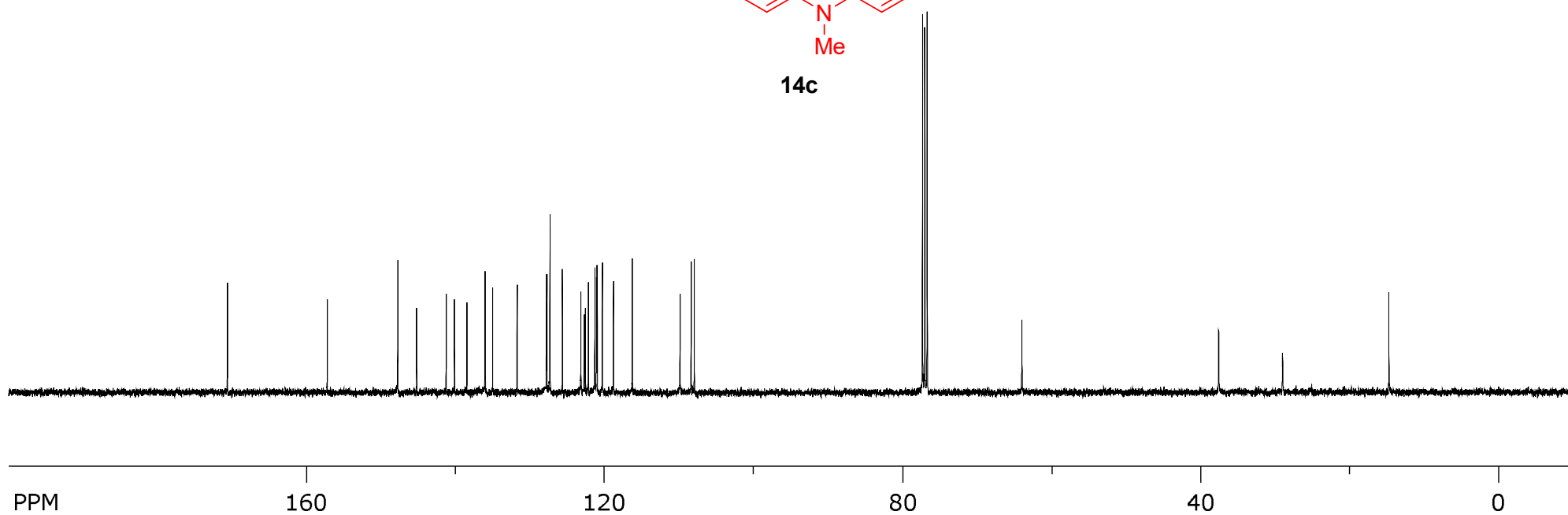


SpinWorks 4: RD-726
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

14.719 —
29.001 —
37.562 —
63.971 —
76.682
77.000
77.318
107.934
108.363
109.850
116.255
118.794
120.284
120.973
121.060
121.284
121.509
125.939
127.313
127.724
127.788
131.718
134.991
136.006
138.447
140.117
141.240
145.194
147.735
157.191
170.586 —

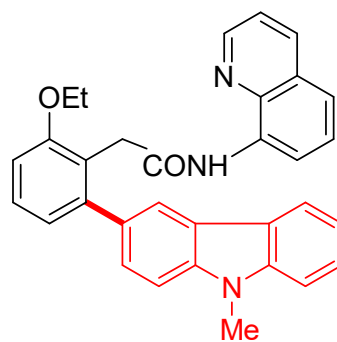


14c

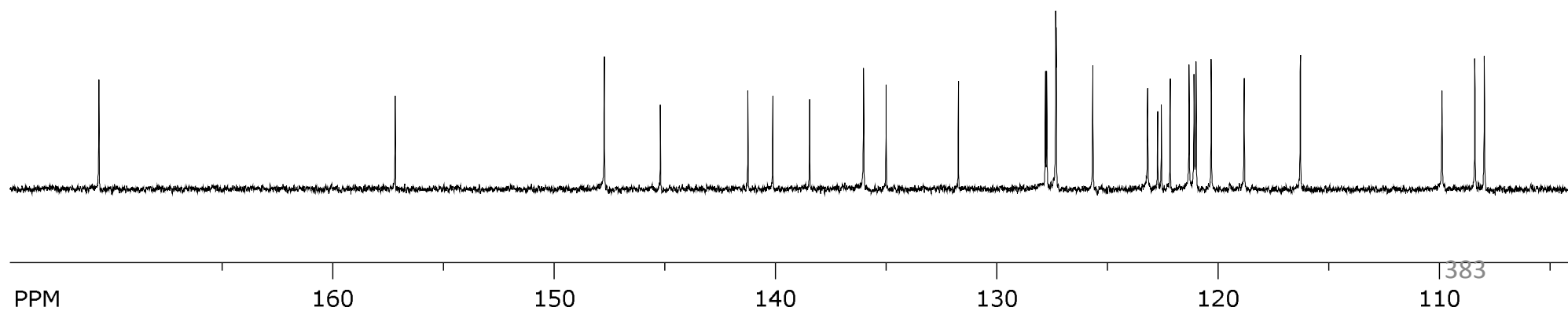


SpinWorks 4: RD-726
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

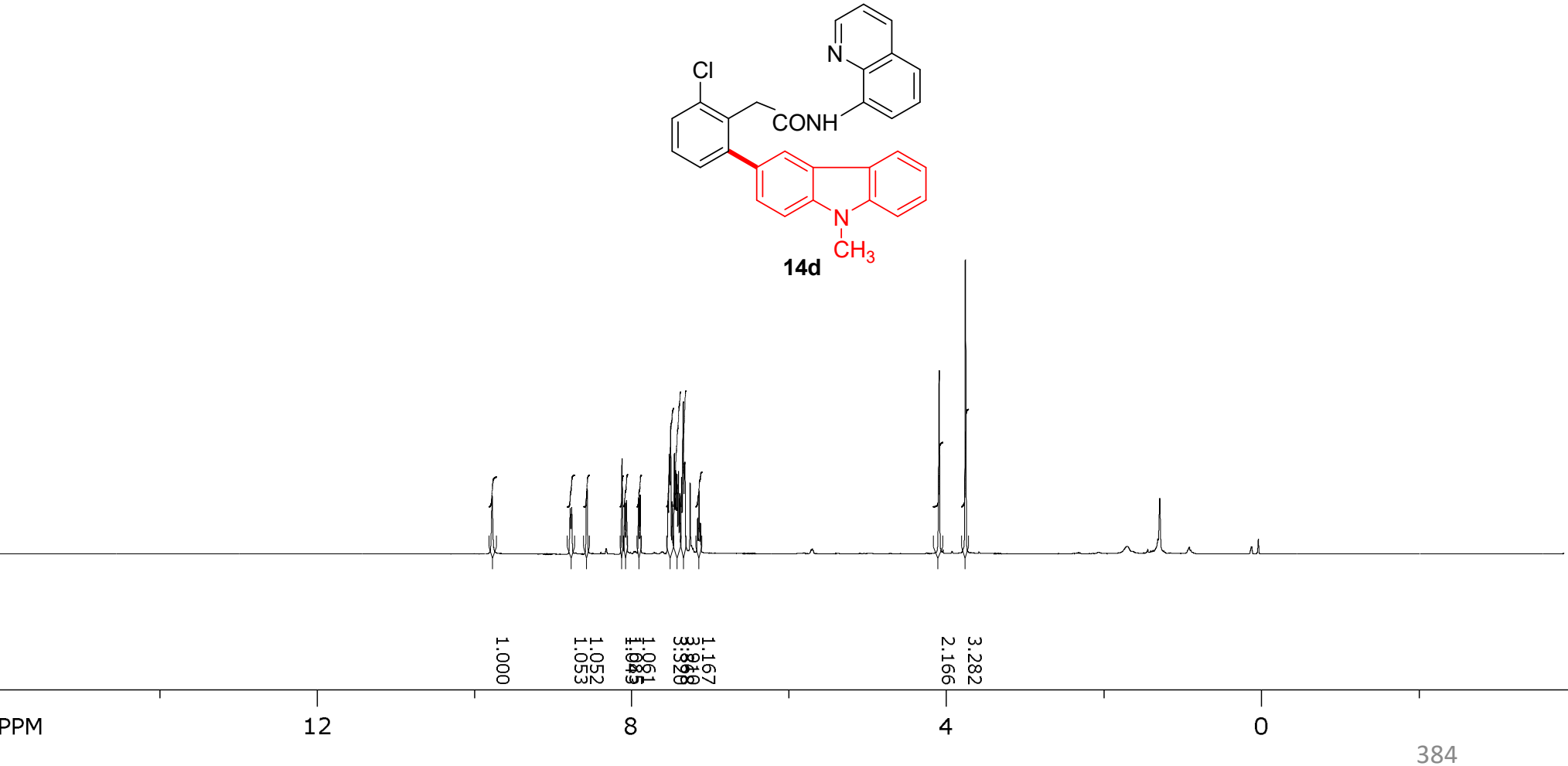
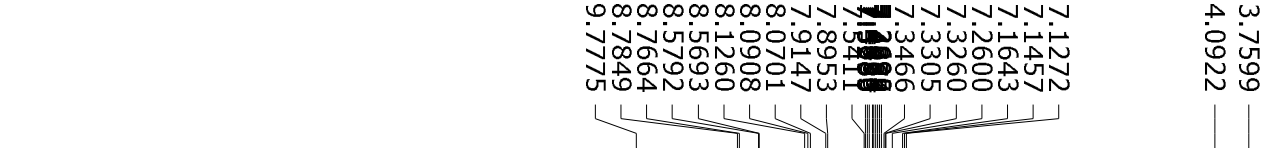
170.586 —
157.191 —
147.735 —
145.194 —
141.240 —
140.117 —
138.447 —
136.006 —
134.991 —
131.718 —
127.788 —
127.724 —
127.315 —
127.293 —
125.639 —
123.163 —
122.710 —
122.540 —
122.145 —
121.284 —
121.060 —
120.973 —
120.284 —
118.794 —
116.255 —
109.850 —
108.363 —
107.934 —



14c

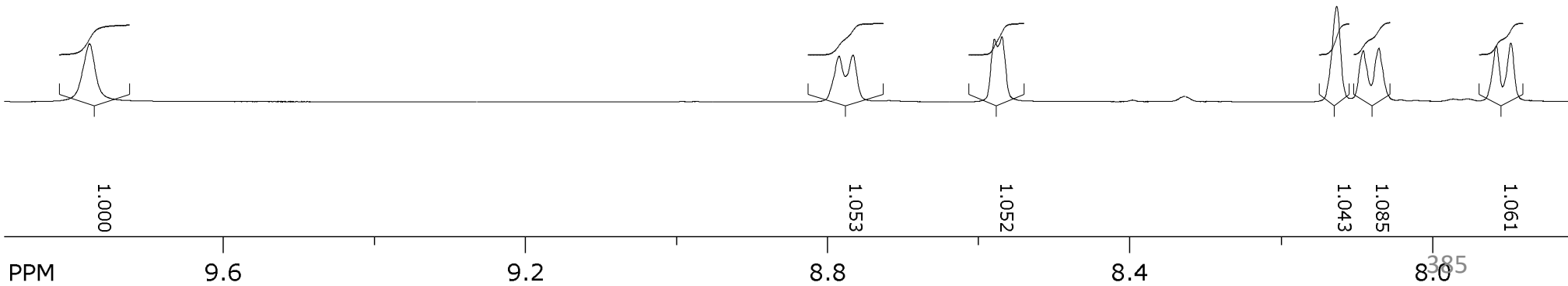
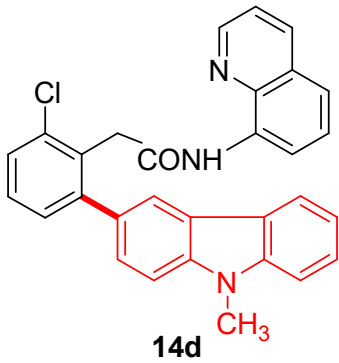


SpinWorks 4: RD 481
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51



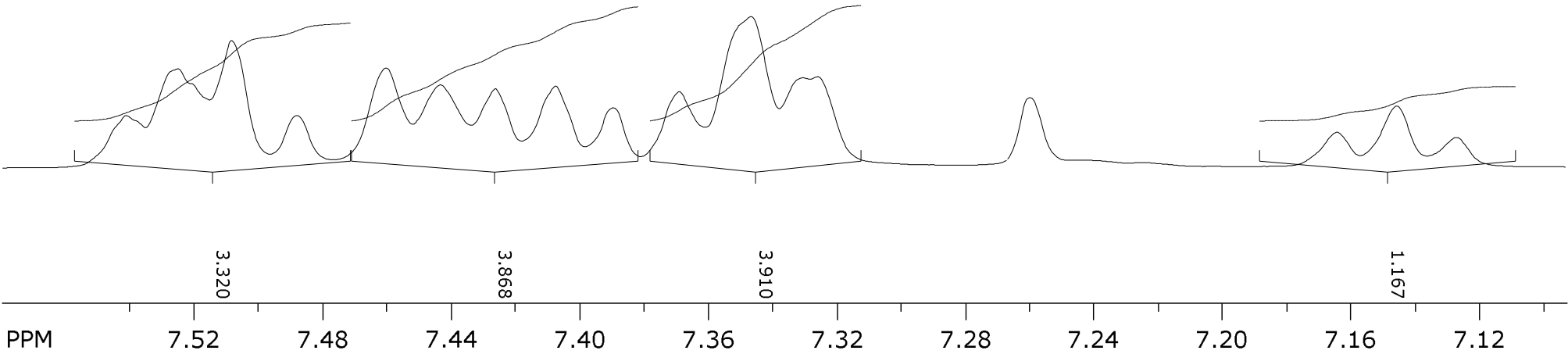
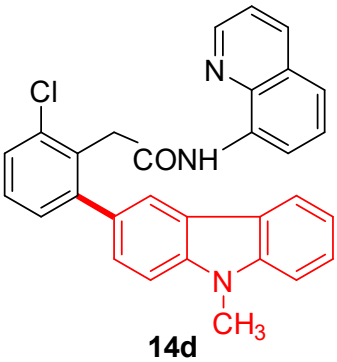
SpinWorks 4: RD 481
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

9.7775 —
8.7664 —
8.7849 —
8.5693 —
8.5792 —
8.0701 —
8.0908 —
8.1260 —
7.8953 —
7.9147 —



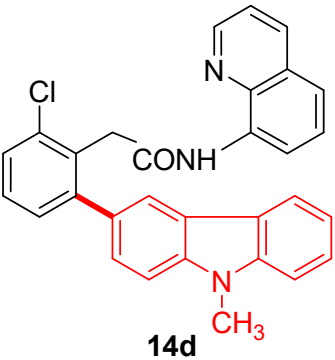
SpinWorks 4: RD 481
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

7.5411 —
7.5250 —
7.5083 —
7.4880 —
7.4603 —
7.4434 —
7.4263 —
7.4074 —
7.3895 —
7.3690 —
7.3466 —
7.3260 —
7.3305 —
7.2600 —
7.1643 —
7.1457 —
7.1272 —

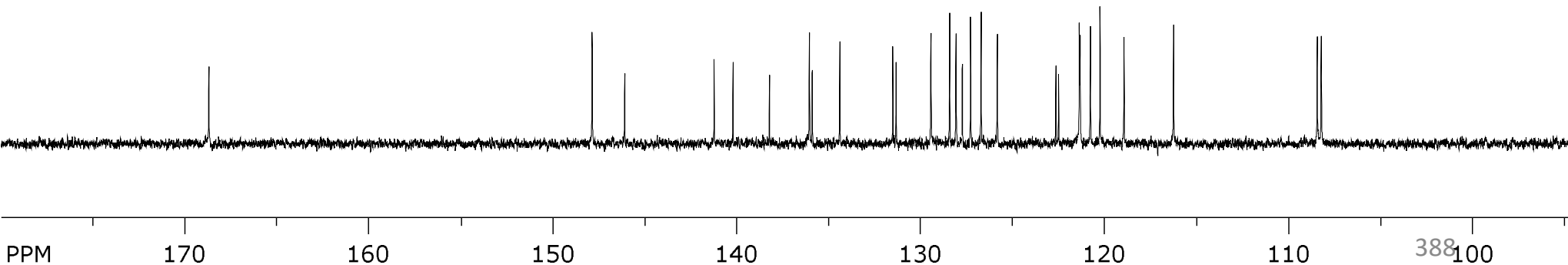
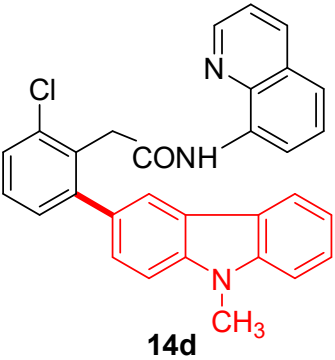
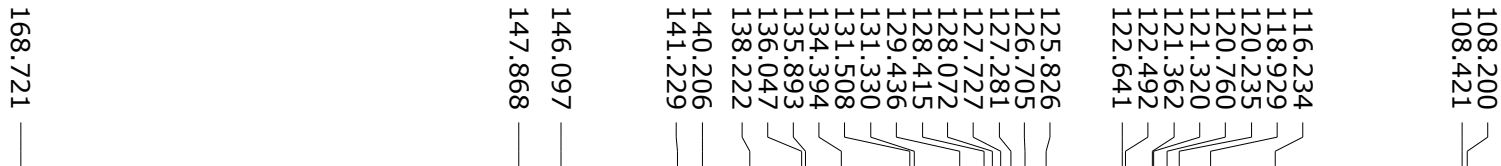


SpinWorks 4: RD 481
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

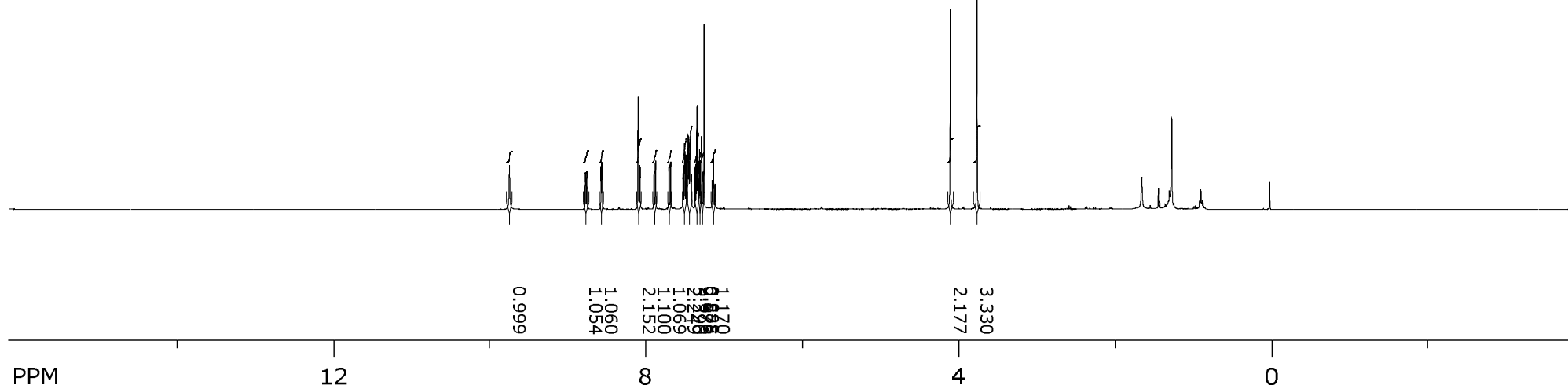
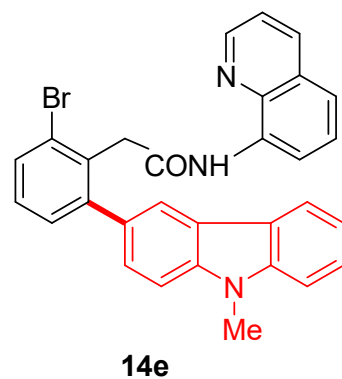
168.721 —
147.868
146.097
141.229
140.206
138.222
136.047
135.893
134.394
131.508
131.330
129.436
129.119
128.836
122.621
121.362
121.320
120.760
120.235
118.929
116.234
108.421
108.200
76.682
77.000
77.318
40.643 —
28.975 —



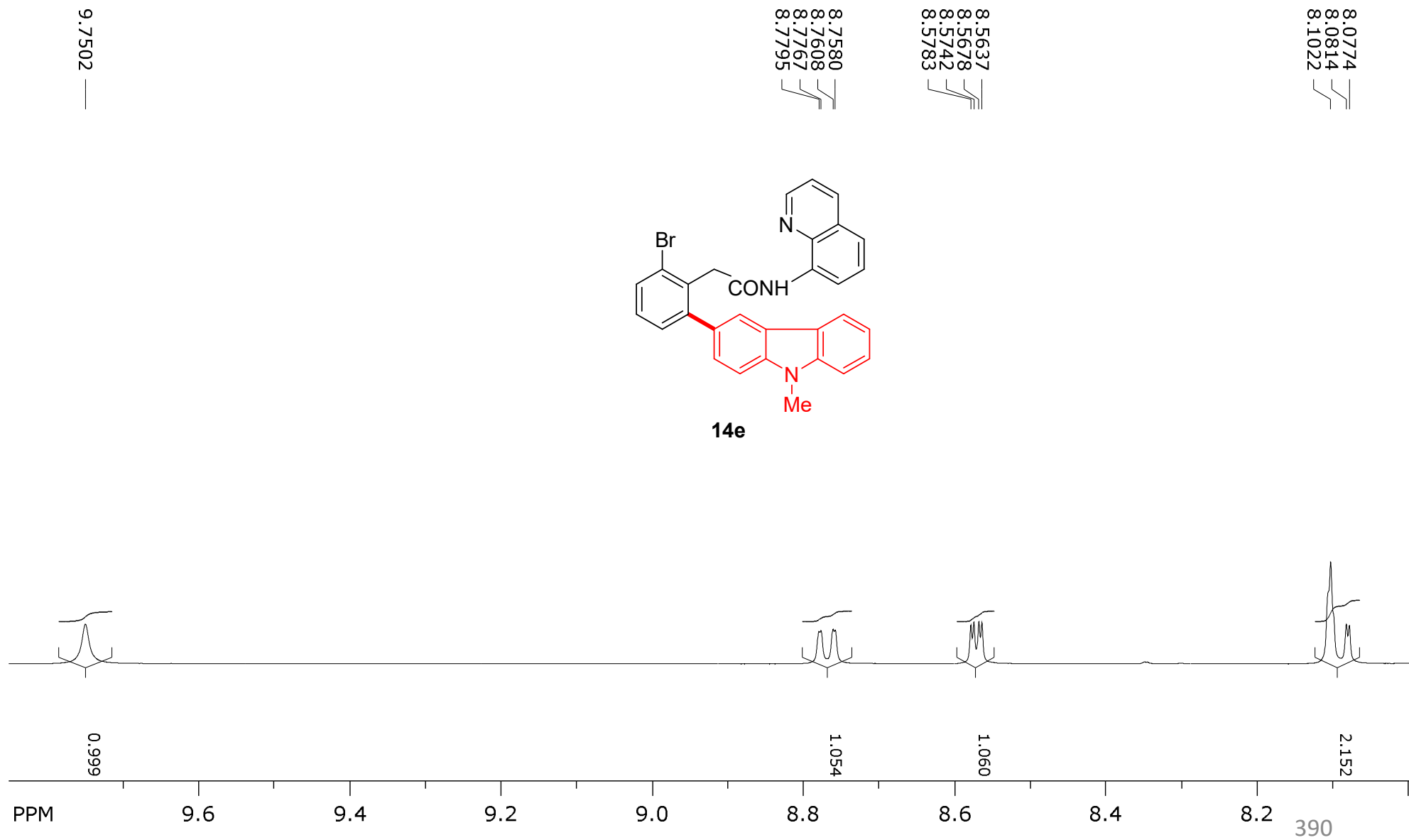
SpinWorks 4: RD 481
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43



SpinWorks 4: RD-2056
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43



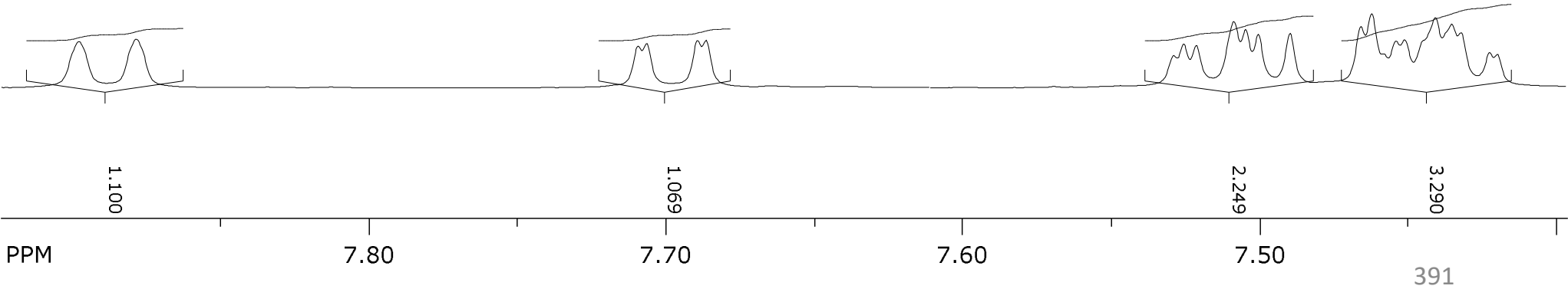
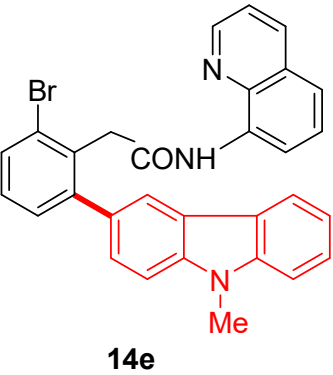
SpinWorks 4: RD-2056
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43

7.8977
7.8784

7.7064
7.7093
7.6864
7.6893

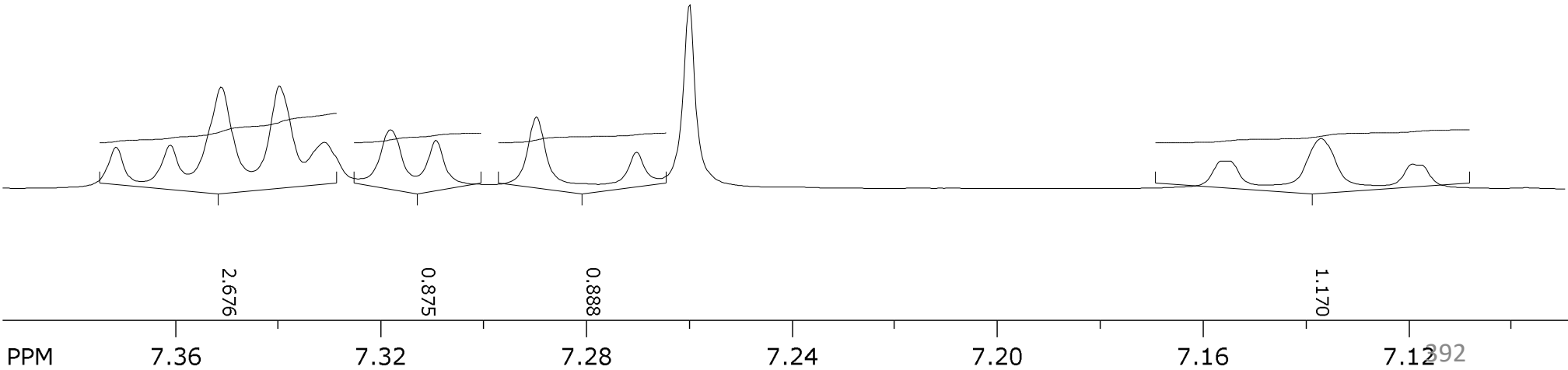
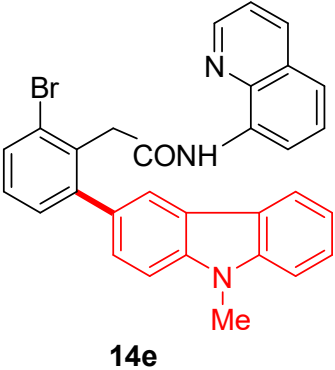
7.5289
7.5255
7.5213
7.5087
7.5047
7.5004
7.4897

7.4658
7.4622
7.4583
7.4540
7.4511
7.4408
7.4353
7.4322
7.4225
7.4199

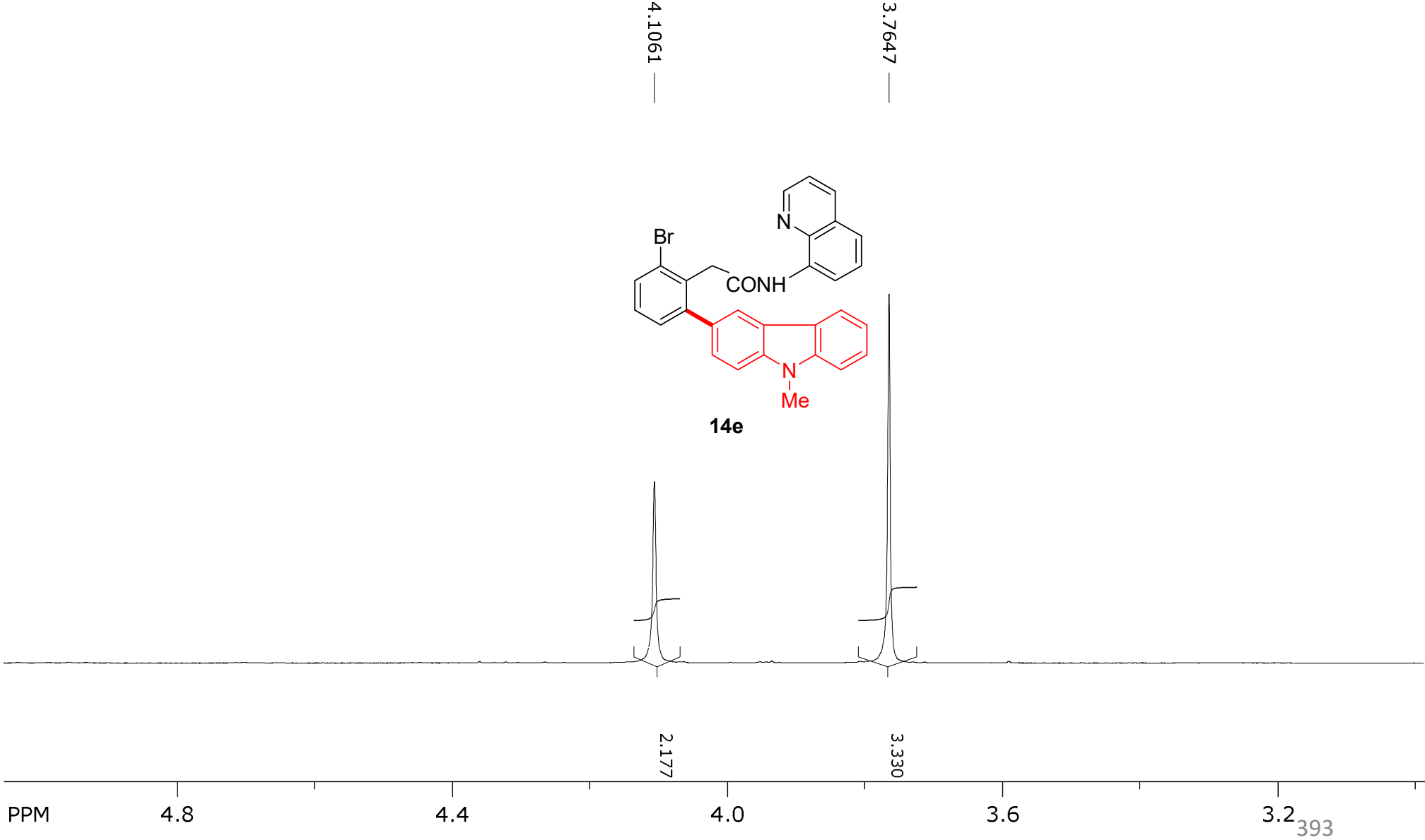


SpinWorks 4: RD-2056
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43

7.3716 —
7.3611 —
7.3512 —
7.3399 —
7.3311 —
7.3182 —
7.3094 —
7.2898 —
7.2703 —
7.2600 —
7.1548 —
7.1563 —
7.1369 —
7.1176 —
7.1192 —



SpinWorks 4: RD-2056
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43



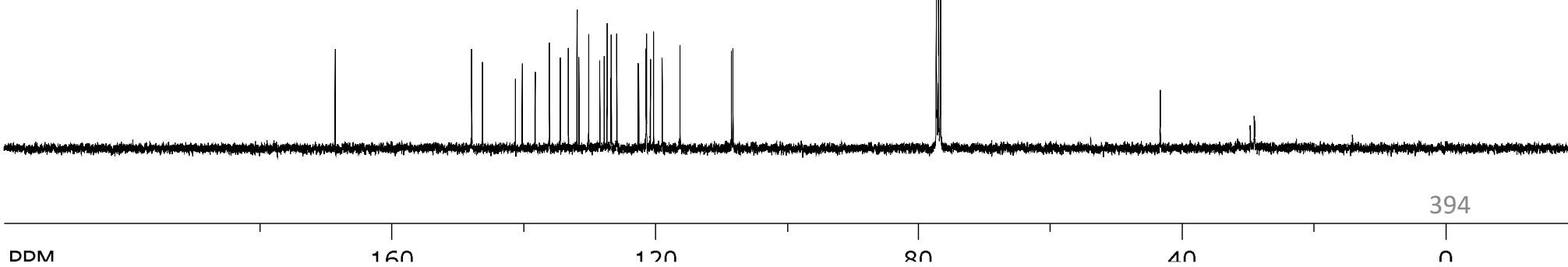
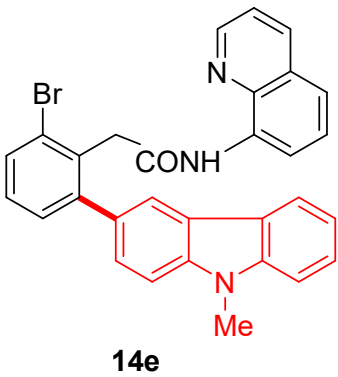
SpinWorks 4: RD-2056
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43

168.632 —
147.897 —
146.255 —
141.257 —
140.232 —
138.264 —
136.083 —
134.437 —
133.211 —
131.899 —
131.606 —
130.466 —
129.959 —
129.957 —
129.955 —
122.639 —
121.397 —
121.335 —
120.755 —
120.267 —
118.957 —
116.255 —
108.445 —
108.217 —

76.703 —
77.020 —
77.338 —

43.340 —

29.021 —



SpinWorks 4: RD-2056

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43

168.632

147.897

146.255

140.232
141.257

138.264

136.083

134.437

133.211

131.899

131.606

130.127

128.429

127.764

127.340

126.797

126.687

125.853

122.639

122.515

121.397

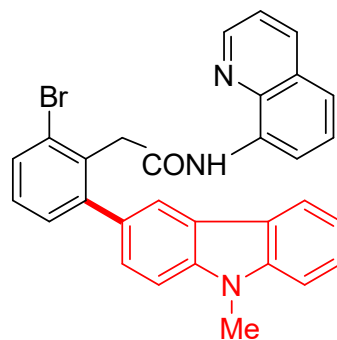
121.335

120.755

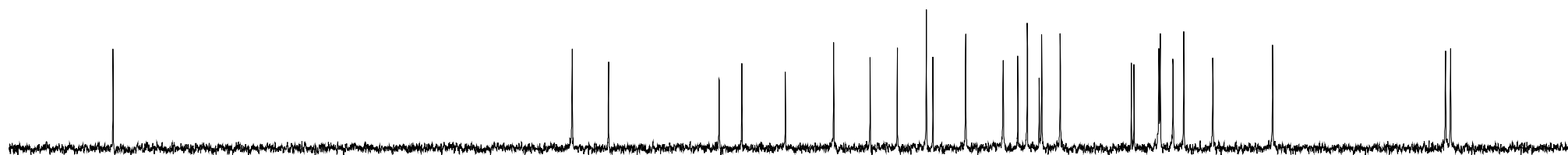
118.957

116.255

108.217
108.445



14e



PPM

160

150

140

130

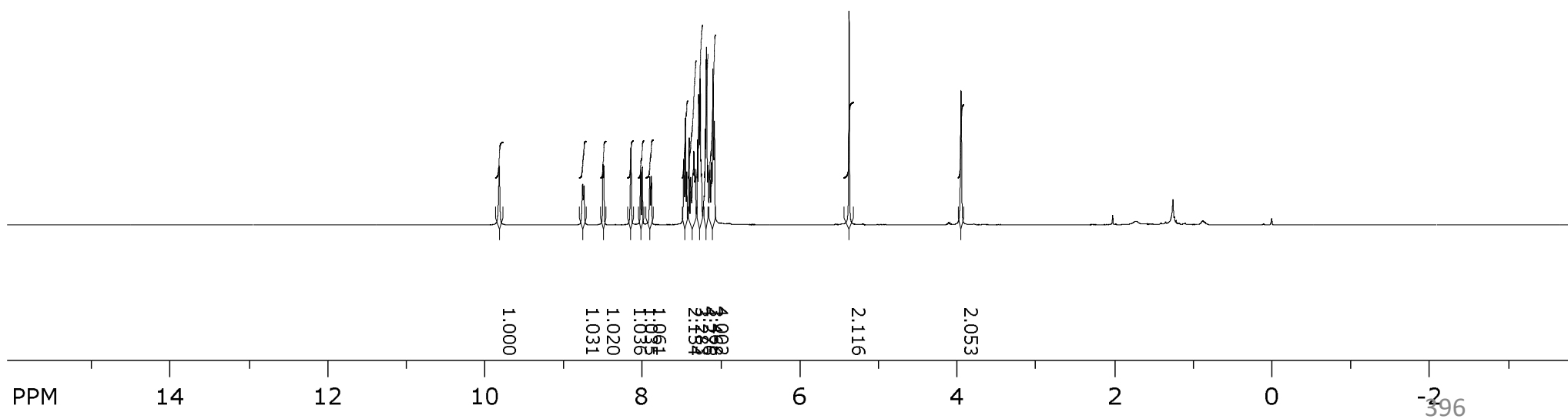
120

110

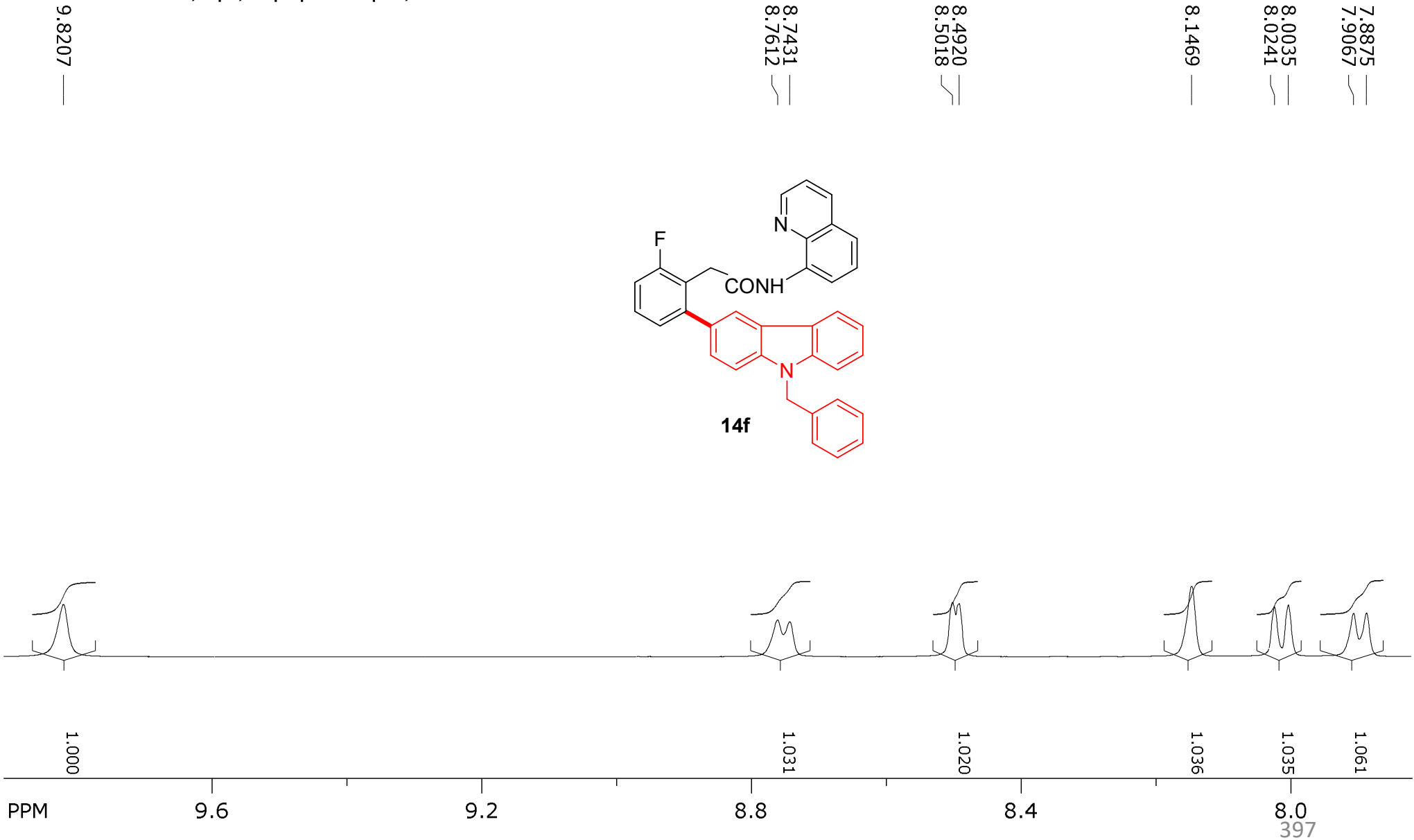
395

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

5.3737
7.0861
7.1043
7.1218
7.1426
7.1673
7.1851
7.1909
7.1958
7.1958
7.8875
7.9067
8.0035
8.0241
8.1469
8.4920
8.5018
8.7431
8.7612
9.8207

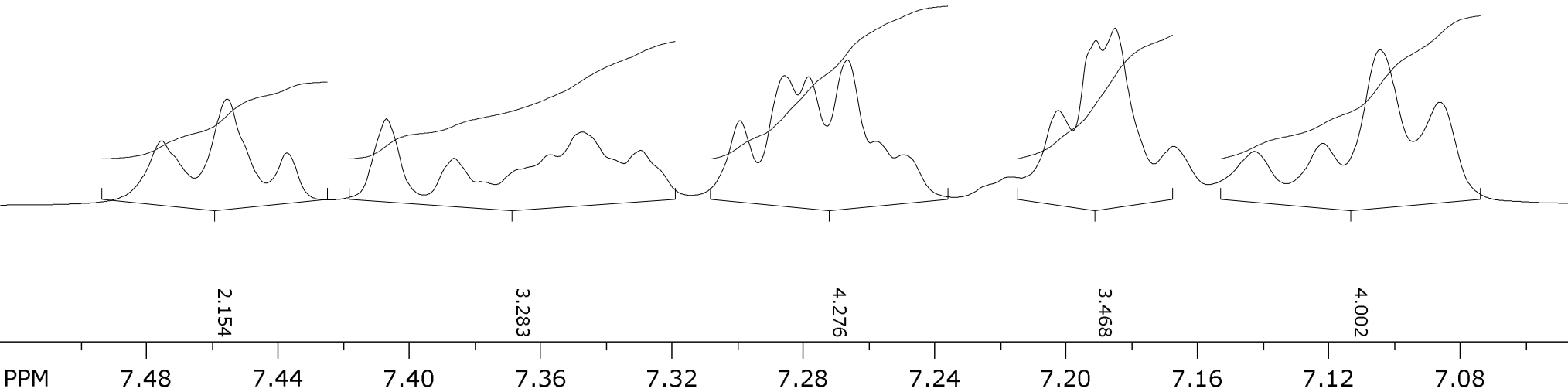
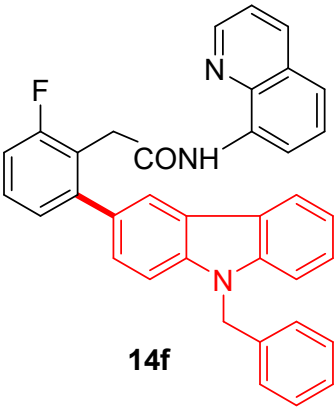


SpinWorks 4: RD 499
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

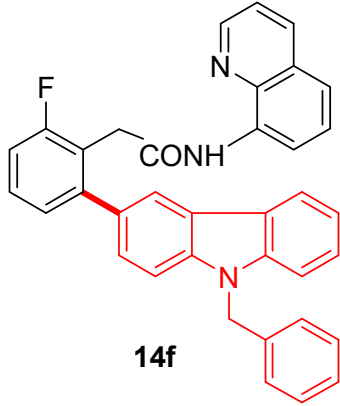
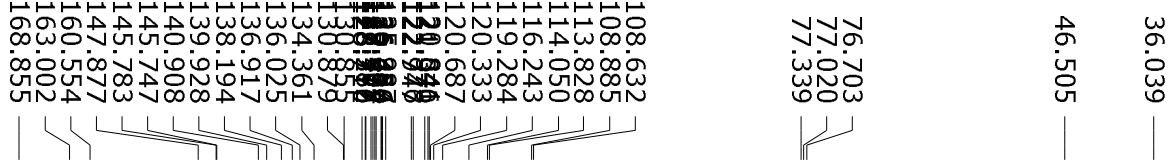


SpinWorks 4: RD 499
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

7.4756 —
7.4557 —
7.4374 —
7.4071 —
7.3865 —
7.3784 —
7.3572 —
7.3474 —
7.3297 —
7.2993 —
7.2858 —
7.2785 —
7.2666 —
7.2581 —
7.2495 —
7.2171 —
7.2024 —
7.1909 —
7.1851 —
7.1673 —
7.1426 —
7.1218 —
7.1043 —
7.0861 —

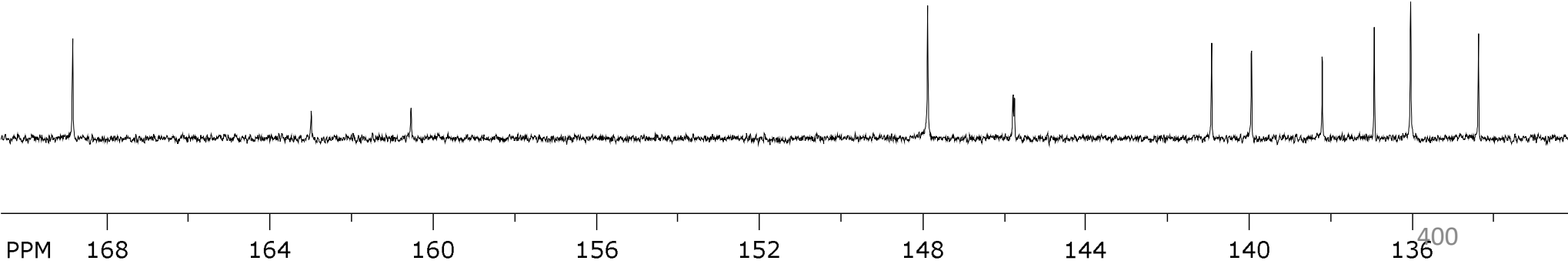
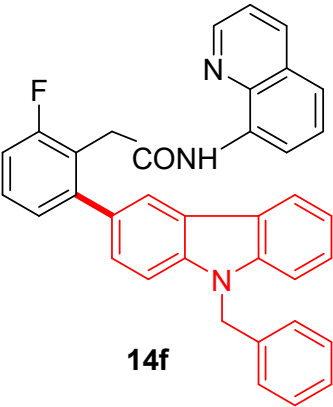


SpinWorks 4: RD 499
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25



PPM 160 120 80 40 0

SpinWorks 4: RD 499
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25



SpinWorks 4: RD 499

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 25

130.855
130.879

128.710
128.376
128.282
127.707
127.427
127.232
127.064
126.480
126.456
126.354
125.987

122.776
122.947

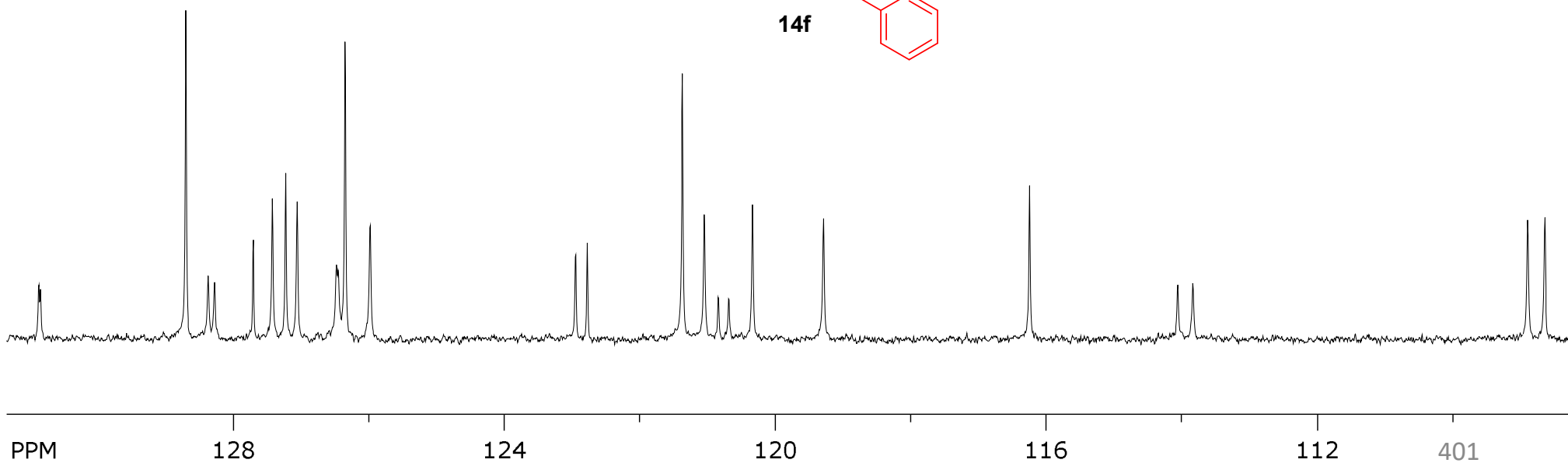
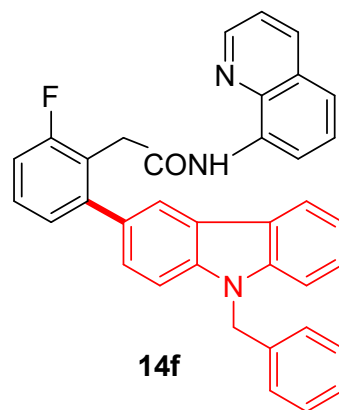
121.370
121.046
120.841
120.687
120.333

119.284

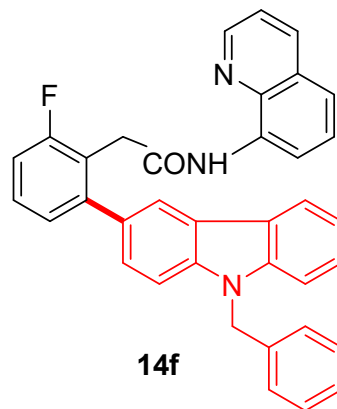
116.243

114.050
113.828

108.885
108.632



SpinWorks 4: RD-499
F19CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 43



-114.2684

PPM

0

-40

-80

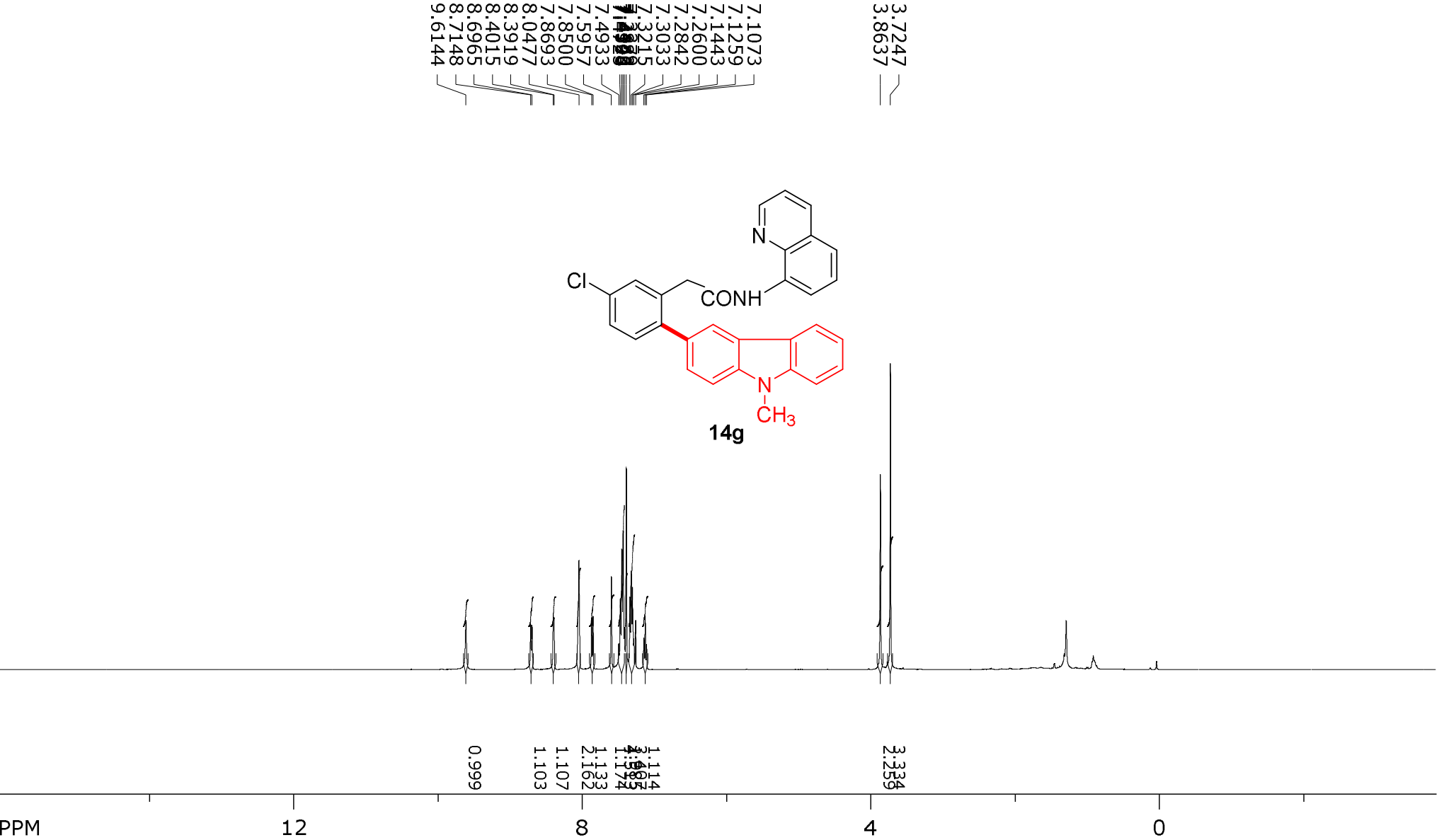
-120

-160

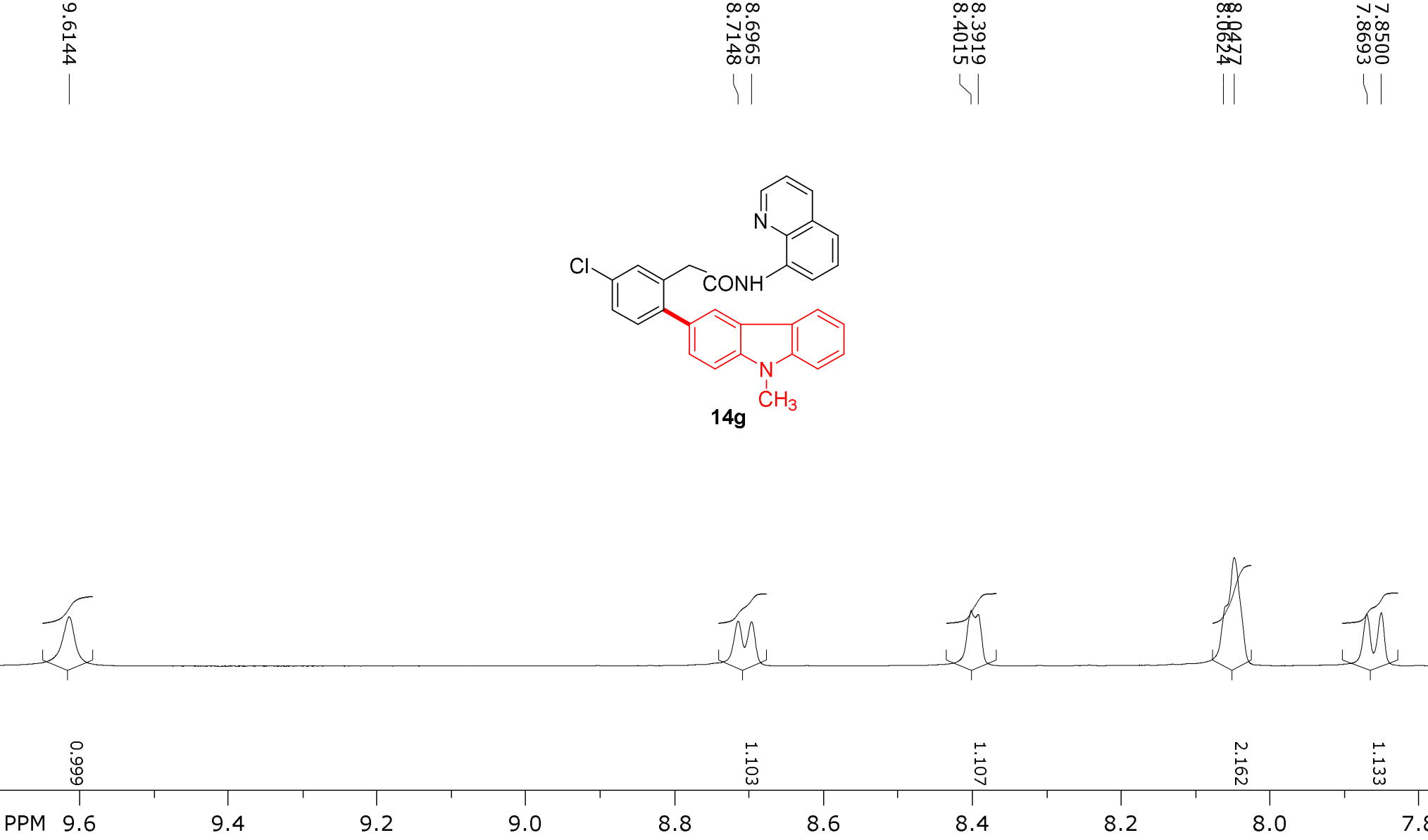
-200

402

SpinWorks 4: RD 526
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

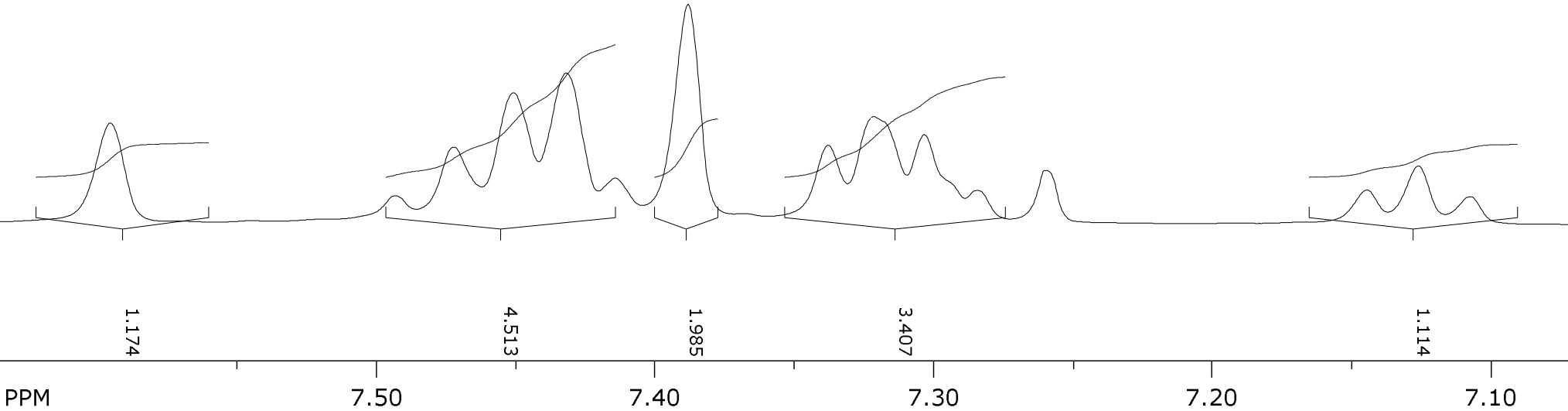
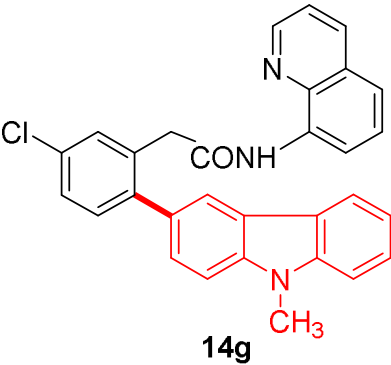


SpinWorks 4: RD 526
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

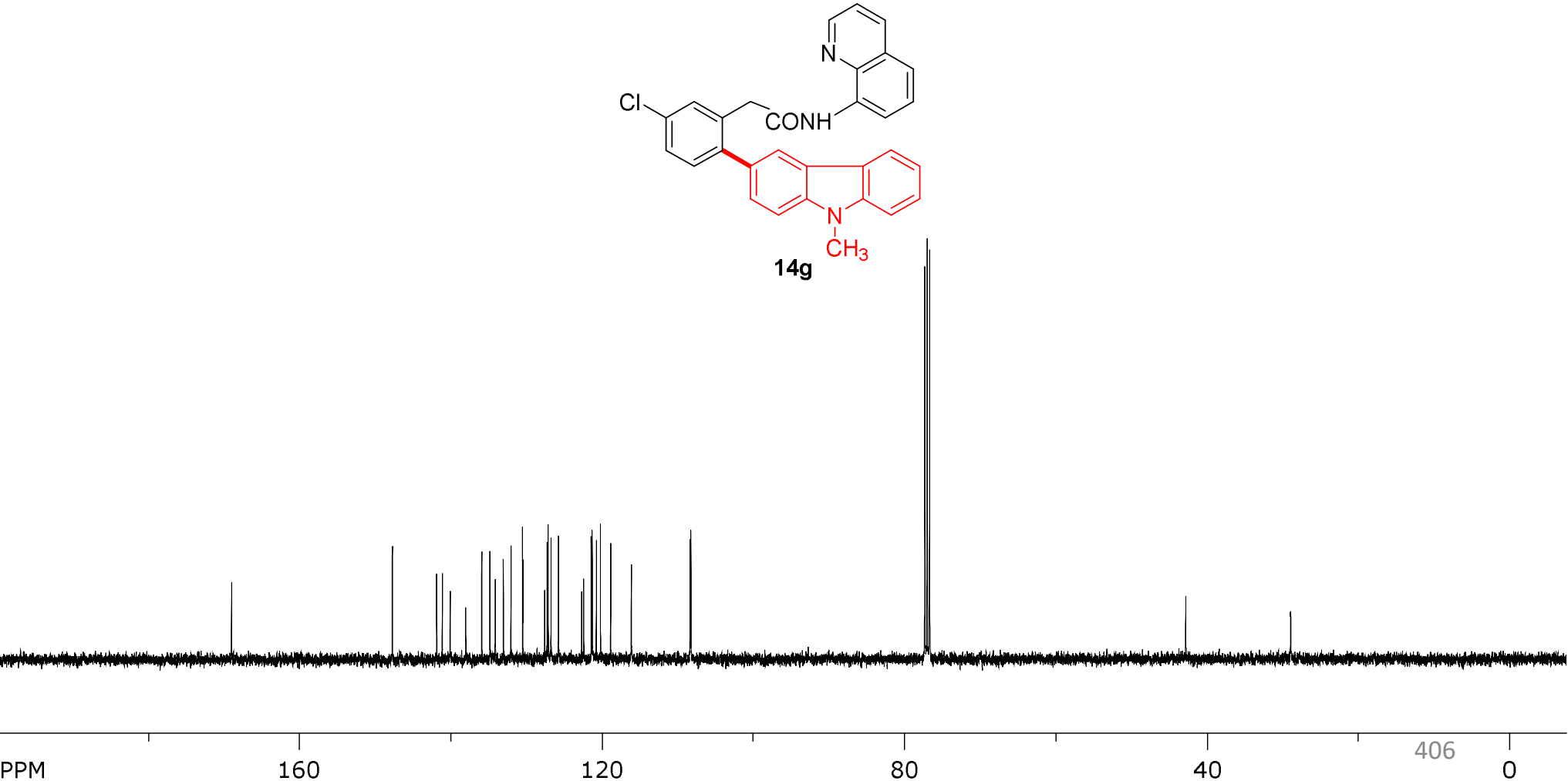


SpinWorks 4: RD 526
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

7.5957 —
7.4933 —
7.4723 —
7.4508 —
7.4320 —
7.4143 —
7.3882 —
7.3379 —
7.3215 —
7.3033 —
7.2842 —
7.2600 —
7.1443 —
7.1259 —
7.1073 —



SpinWorks 4: RD 526
13C



SpinWorks 4: RD 526
13C

169.033

147.758

140.112

141.150

141.894

138.039

135.929

134.857

134.151

133.063

132.068

130.525

130.482

127.598

127.286

127.137

126.773

125.781

122.722

122.439

121.443

121.309

120.772

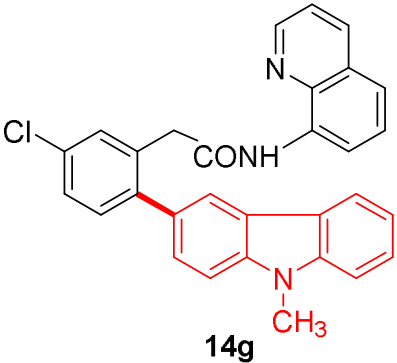
120.224

118.876

116.142

108.359

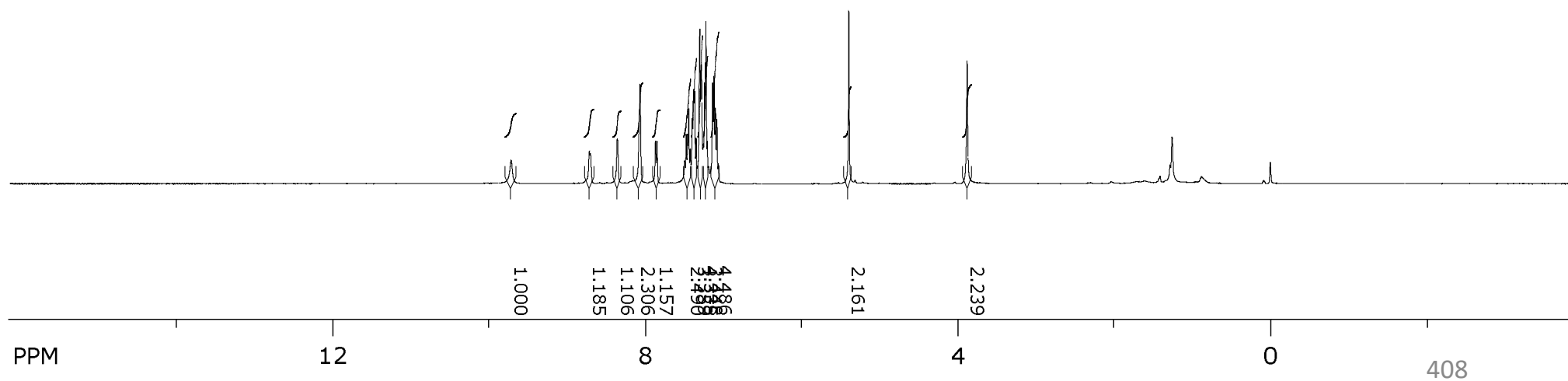
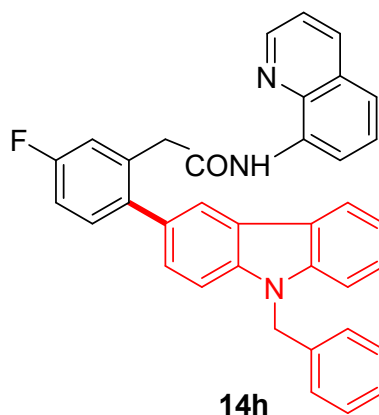
108.251



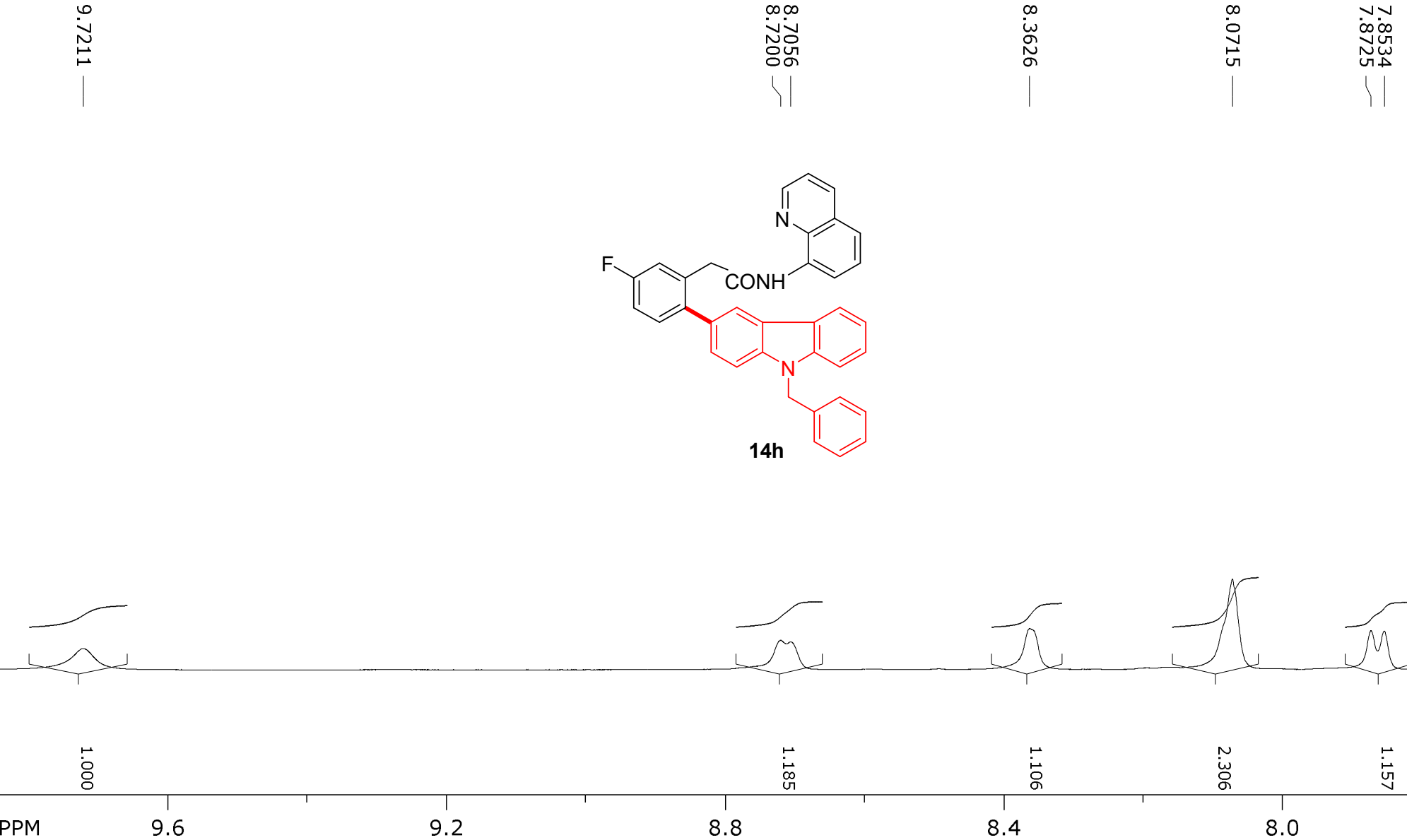
PPM 170 160 150 140 130 120 110 407

SpinWorks 4: RD 530
1H

3.8834
5.3976
7.0636
7.0682
7.0884
7.1056
7.1235
7.1419
7.1905
7.1910
7.1915
7.1920
7.1925
7.4475
7.4797
7.4998
7.8534
7.8725
8.0715
8.3626
8.7056
8.7200
9.7211
9.7217

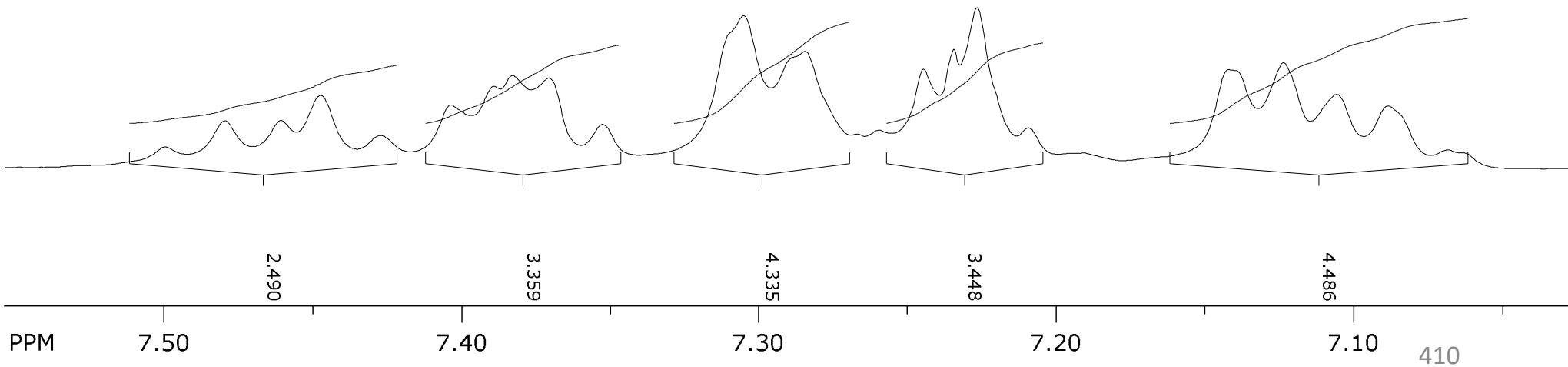
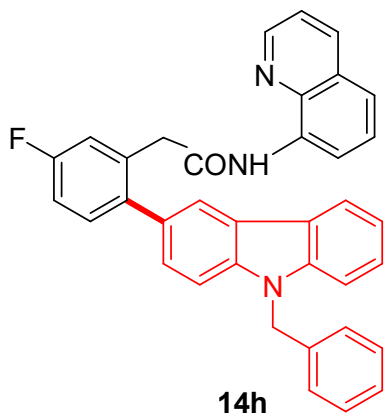


SpinWorks 4: RD 530
1H



SpinWorks 4: RD 530
1H

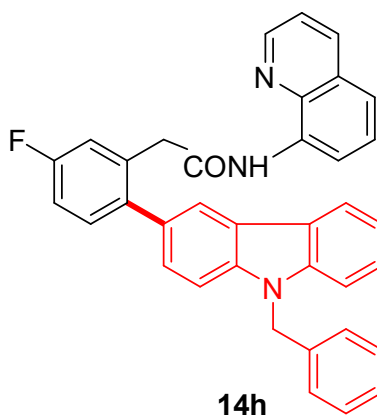
7.4998 —
7.4797 —
7.4475 —
7.4274 —
7.4037 —
7.3828 —
7.3891 —
7.3706 —
7.3526 —
7.3051 —
7.2844 —
7.2670 —
7.2596 —
7.2446 —
7.2344 —
7.2266 —
7.2094 —
7.1905 —
7.1946 —
7.1419 —
7.1235 —
7.1056 —
7.0884 —
7.0636 —
7.0682 —



SpinWorks 4: RD-530

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29

108.692
108.872
114.026
114.227
117.125
117.339
119.274
120.387
121.898
122.811
124.198
125.970
126.970
128.970
131.313
132.393
133.089
135.107
137.004
139.350
139.381
139.852
140.940
147.621
160.787
163.235
169.311
77.338
77.020
76.703
46.596
42.951



PPM

160

120

80

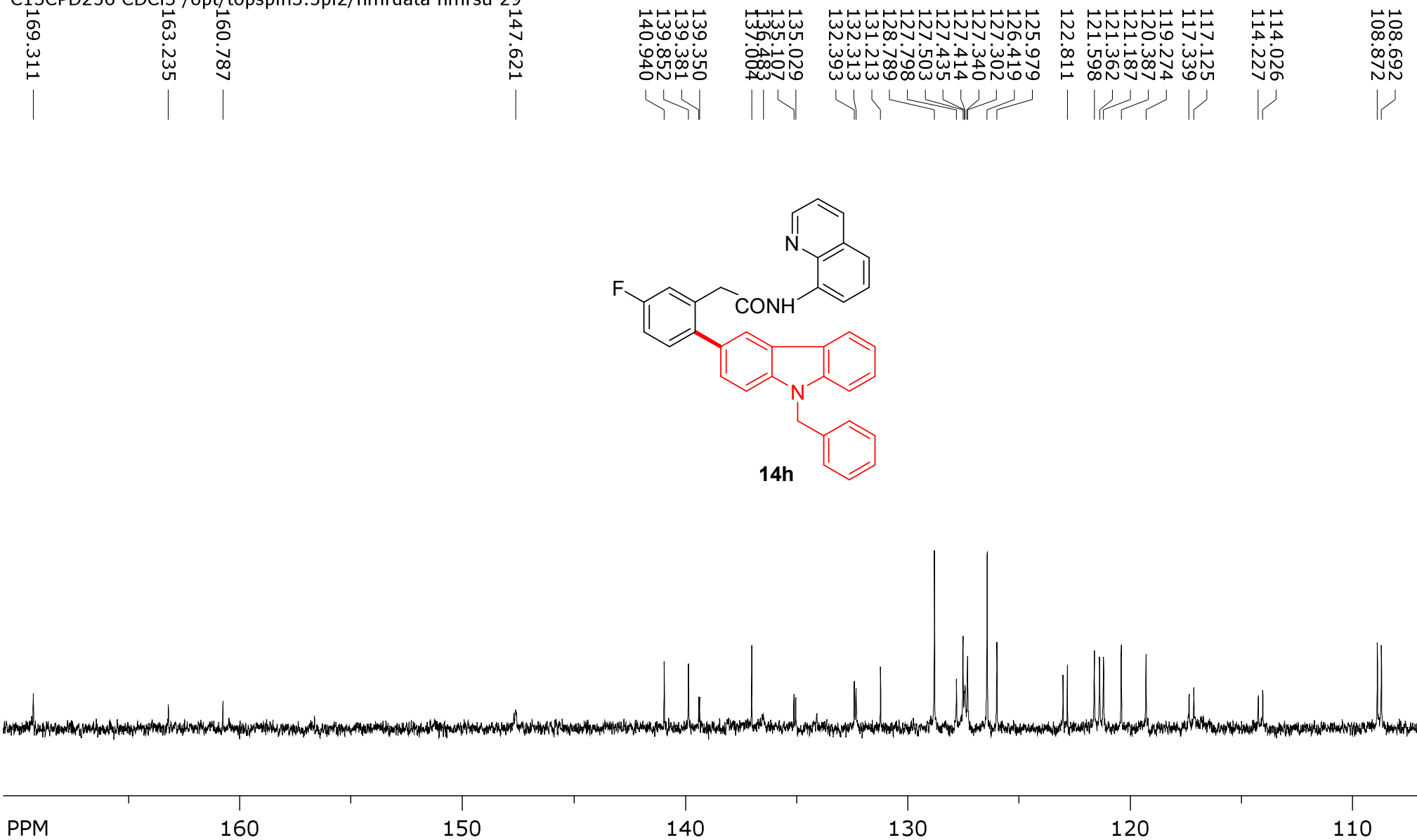
40

0

411

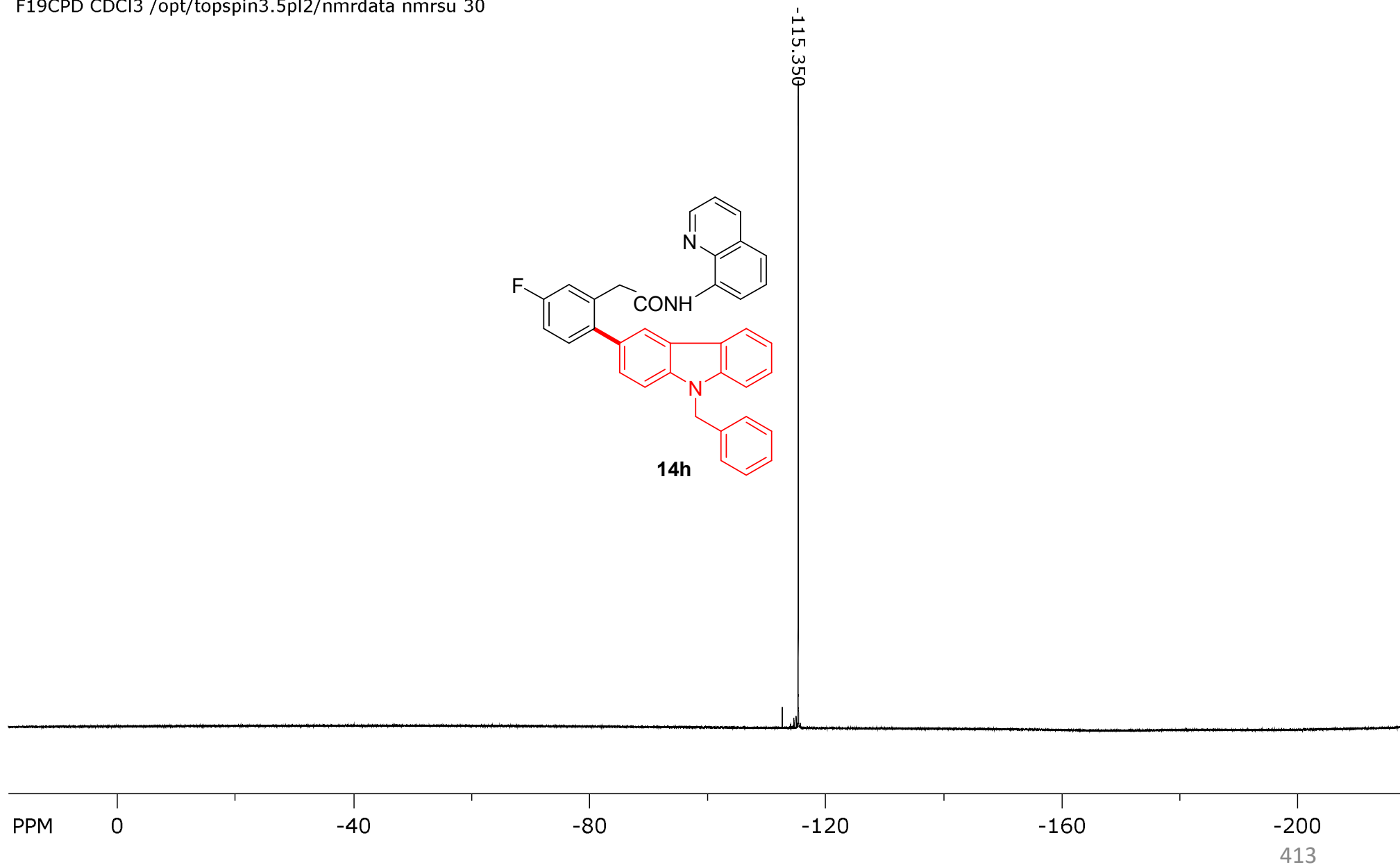
SpinWorks 4: RD-530

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29

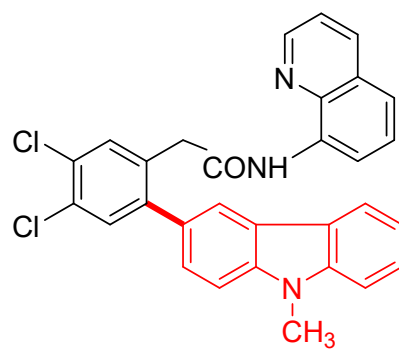


SpinWorks 4: RD-530

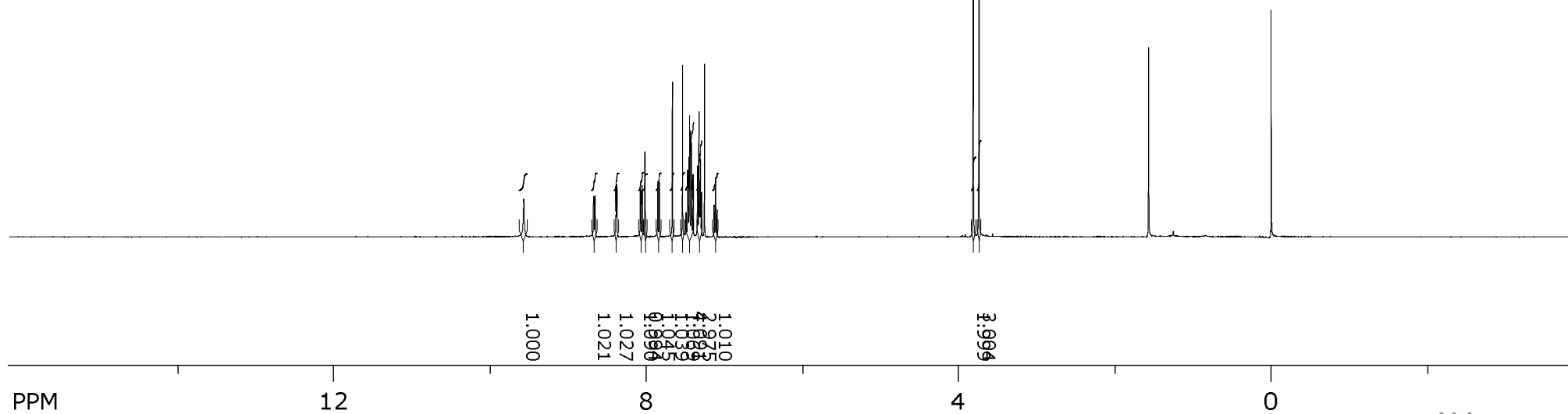
F19CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8



14i



SpinWorks 4: RD 742

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

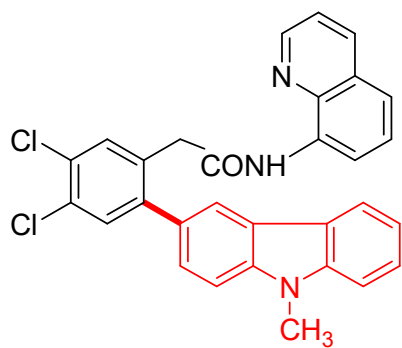
9.5705

8.6560
8.6601
8.6740
8.6780

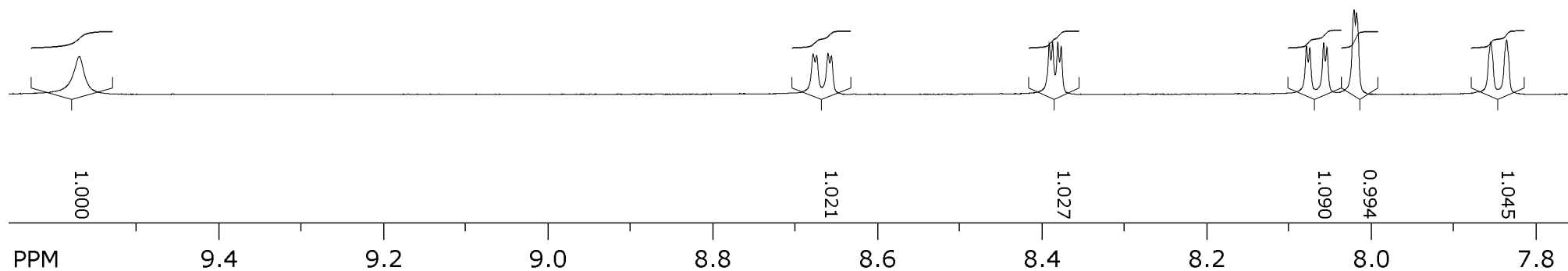
8.3767
8.3808
8.3872
8.3913

8.0174
8.0203
8.0536
8.0577
8.0743
8.0784

7.8350
7.8544



14i



SpinWorks 4: RD 742

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

7.6678

7.5378

7.4926

7.4716

7.4669

7.4534

7.4466

7.4430

7.4256

7.4214

7.4045

7.4003

7.3449

7.3269

7.3155

7.3063

7.2949

7.2566

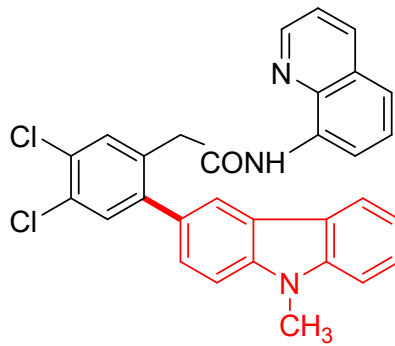
7.1347

7.1329

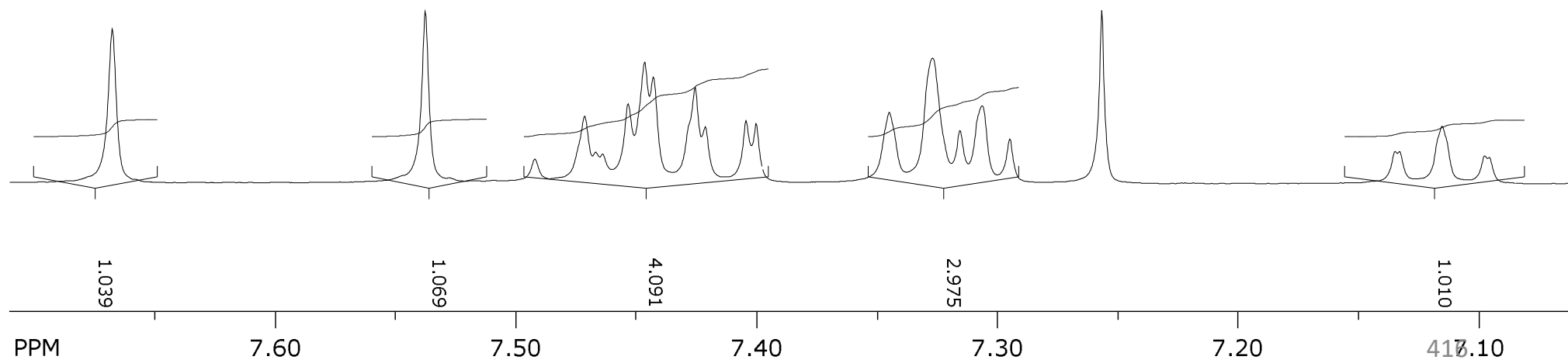
7.1152

7.0980

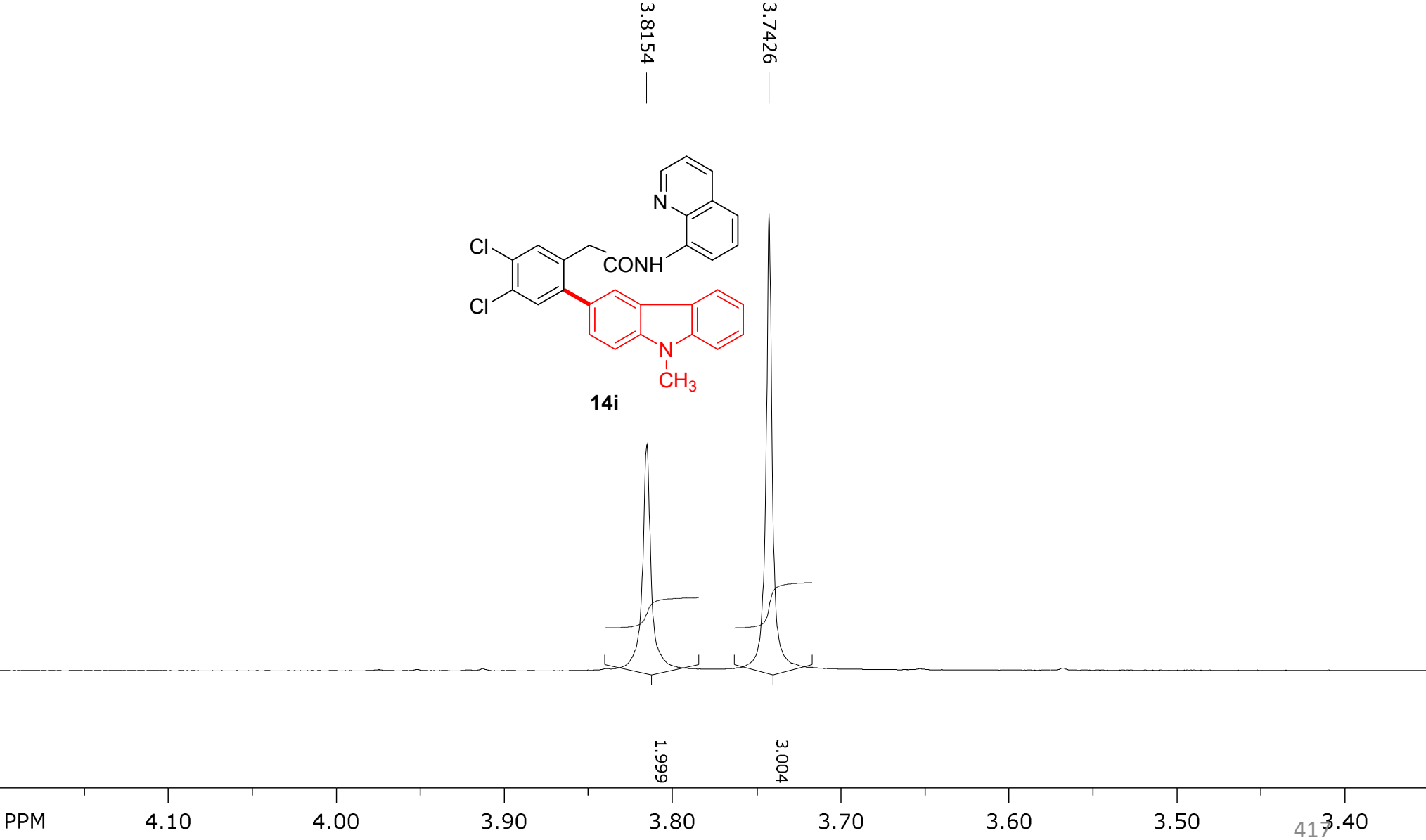
7.0942



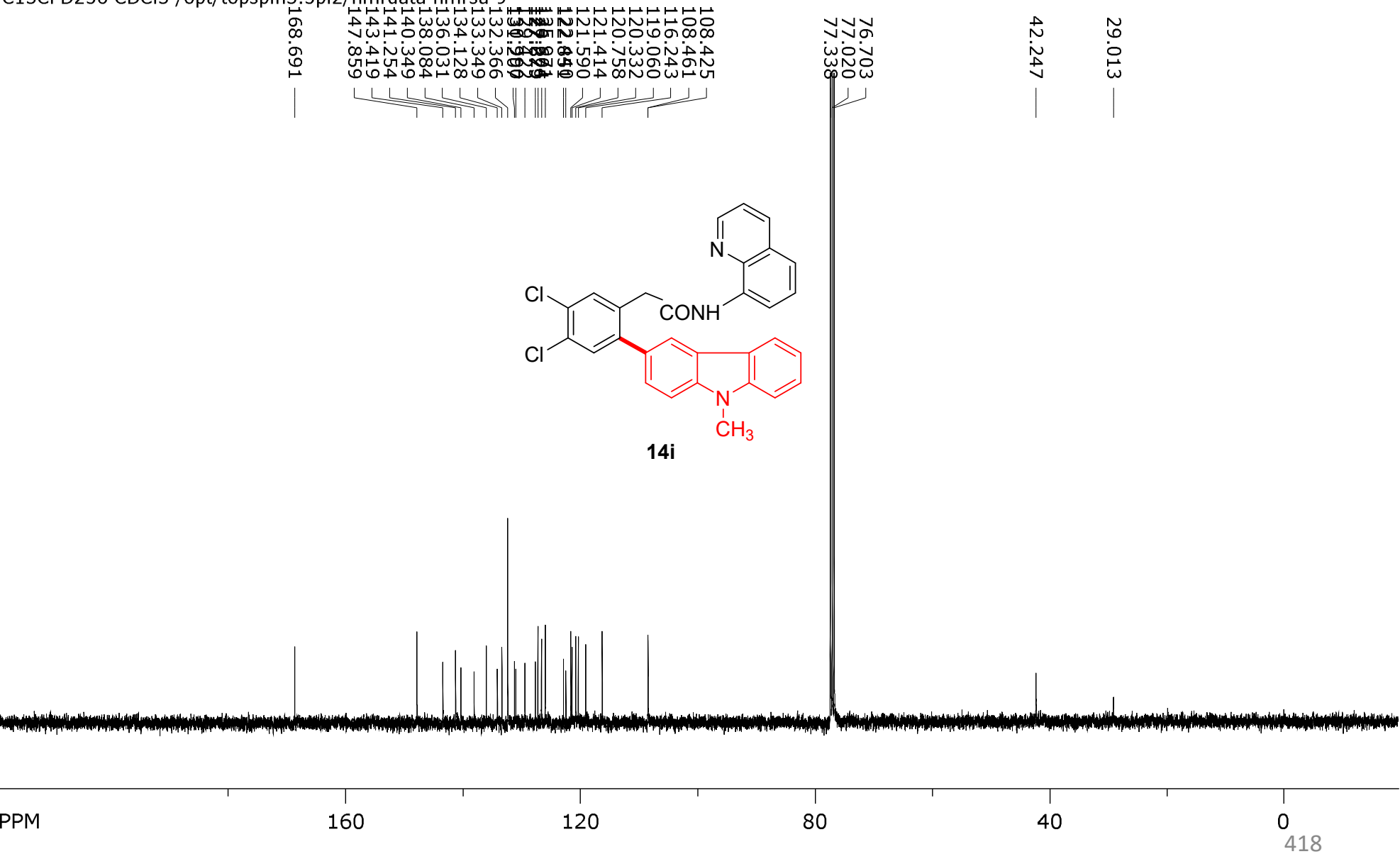
14i



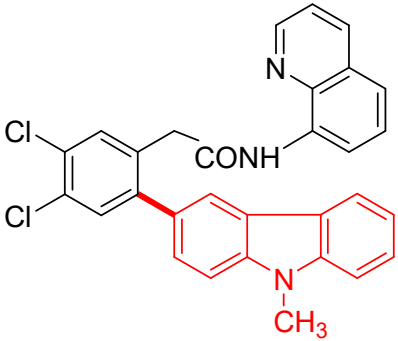
SpinWorks 4: RD 742
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8



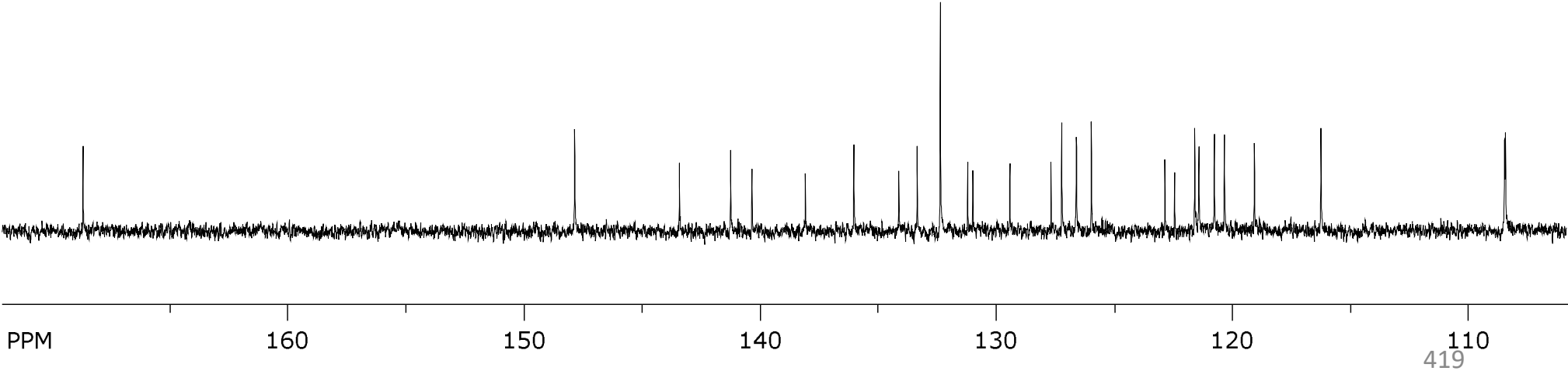
SpinWorks 4: RD 742
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9



SpinWorks 4: RD 742
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

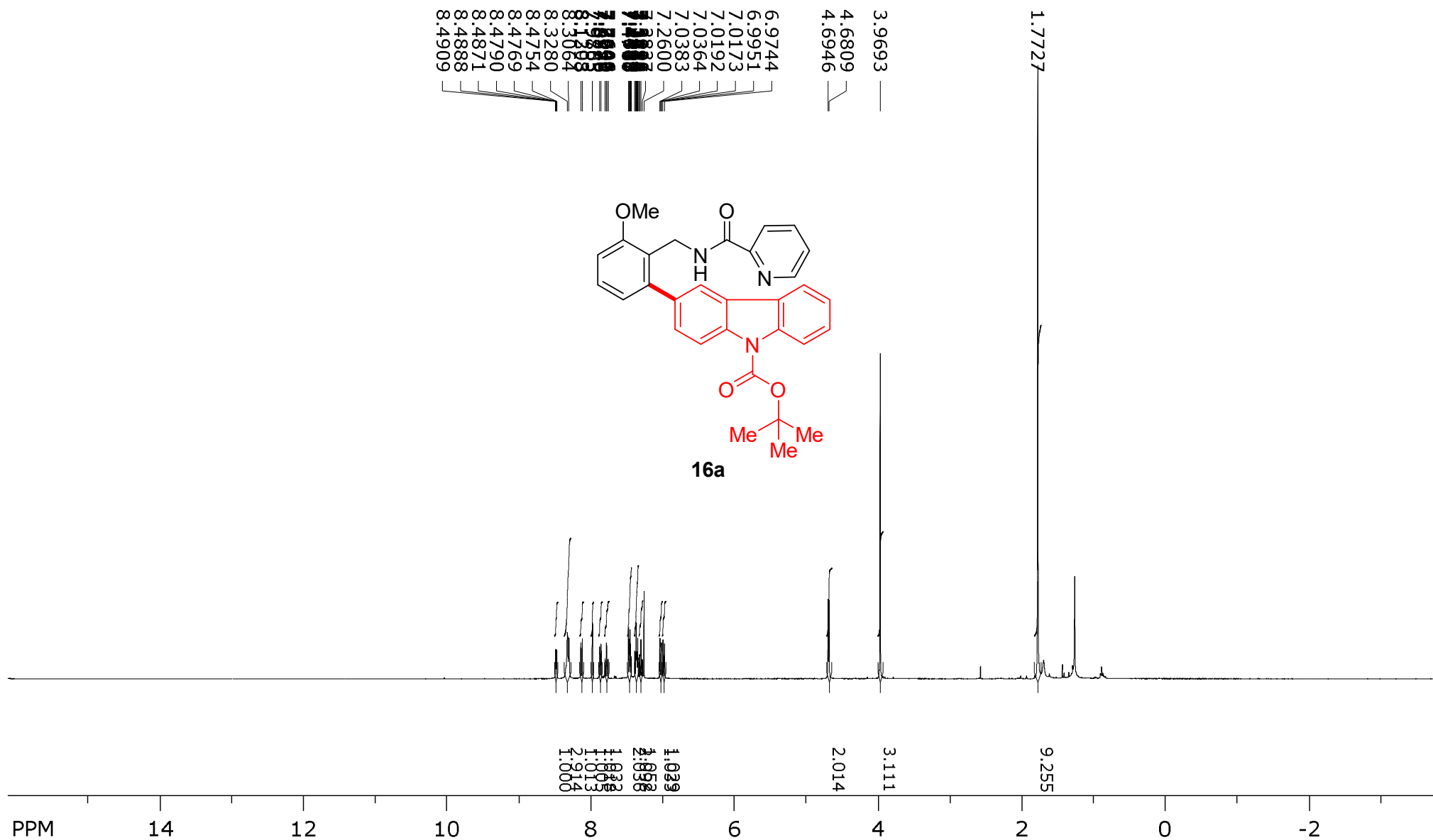


14i



SpinWorks 4: RD-1169

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 5



SpinWorks 4: RD-1169
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

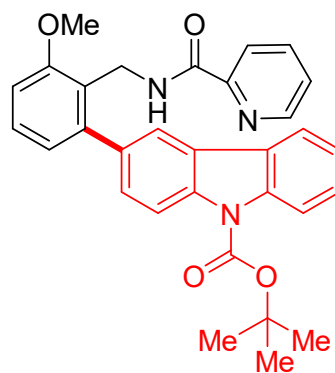
8.4754
8.4769
8.4790
8.4871
8.4888
8.4909

8.3280
8.3064

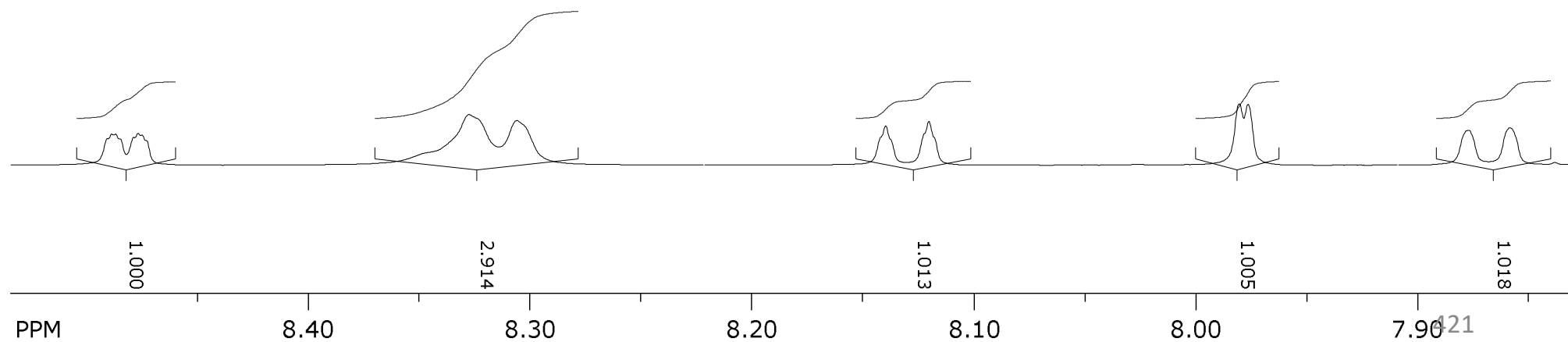
8.1398
8.1203

7.9765
7.9805

7.8776
7.8586



16a



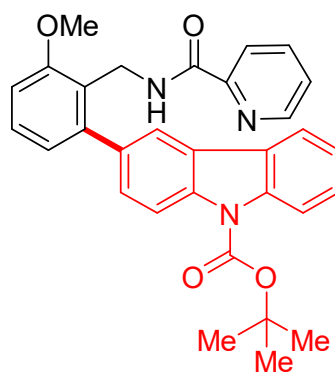
SpinWorks 4: RD-1169

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

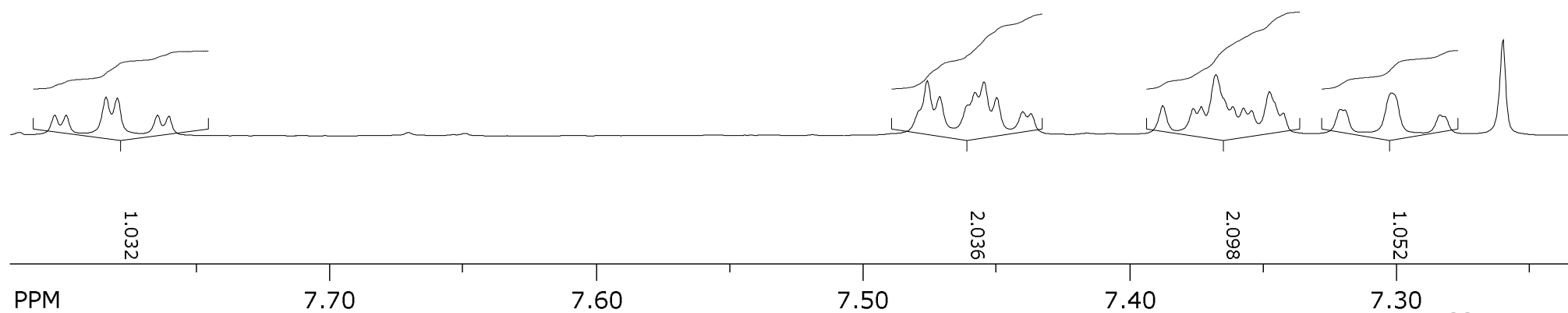
7.7696
7.7696
7.7799
7.7841
7.7990
7.8033

7.4371
7.4401
7.4499
7.4547
7.4580
7.4608
7.4713
7.4760

7.3876
7.3761
7.3731
7.3678
7.3613
7.3573
7.3543
7.3476
7.3424
7.3211
7.3195
7.3020
7.2837
7.2600

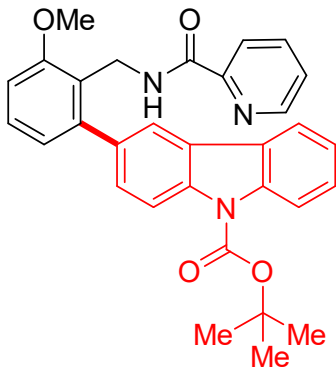


16a

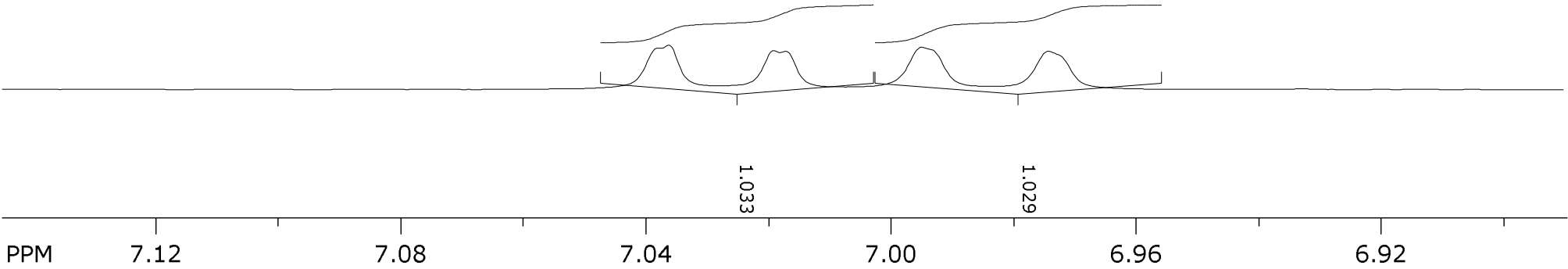


SpinWorks 4: RD-1169
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

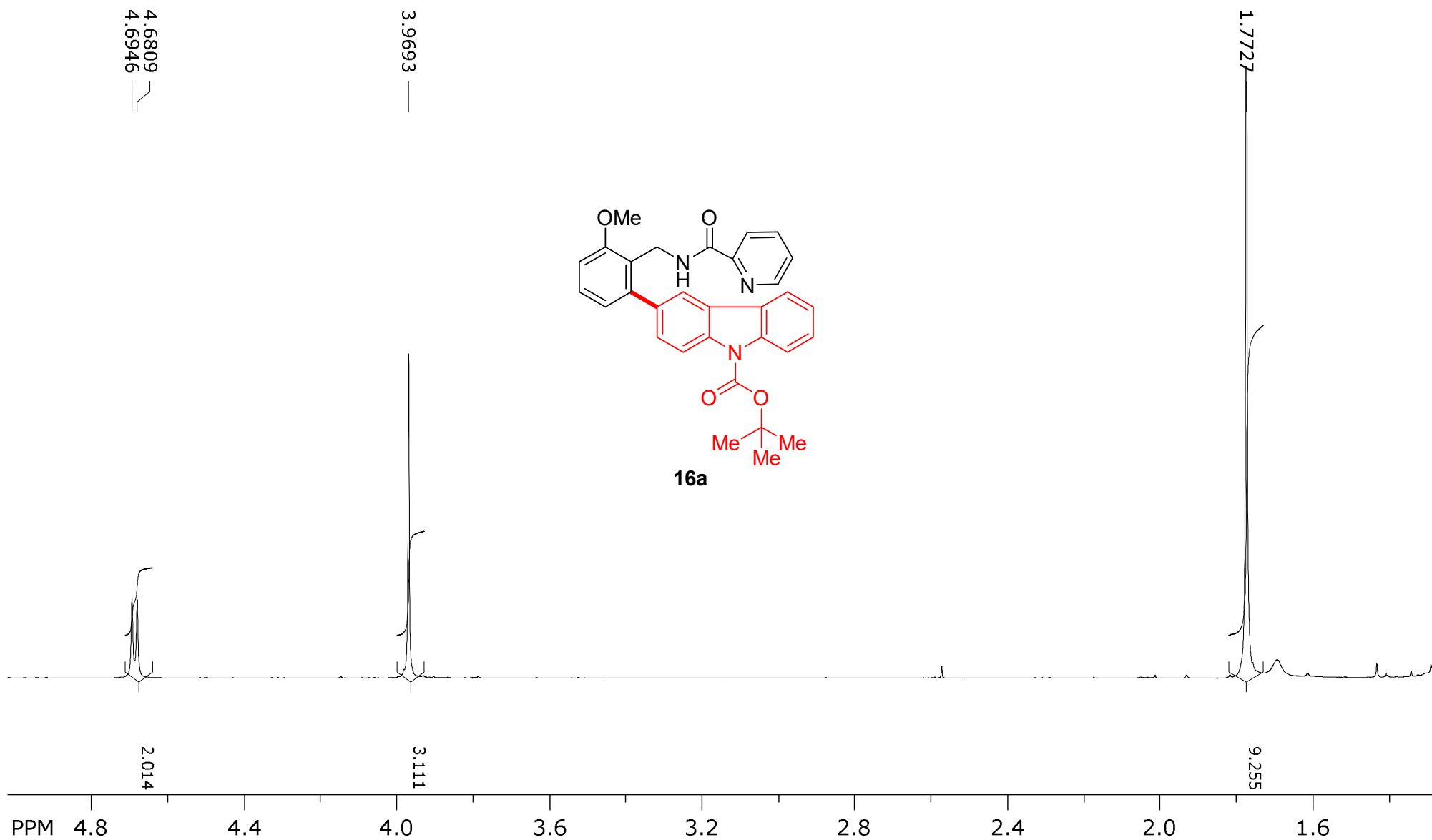
7.0364
7.0383
7.0173
7.0192
6.9951
6.9744



16a



SpinWorks 4: RD-1169
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5



SpinWorks 4: RD-1169

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

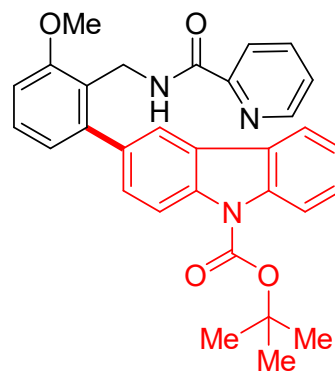
109.554
116.022
116.238
119.698
120.359
122.185
122.934
123.061
123.912
125.809
125.819
127.097
128.166
128.394
135.395
137.122
137.702
138.897
144.066
147.960
150.272
151.087
158.658
163.295

83.909
77.337
77.020
76.702

55.887

36.685

28.380



16a

PPM

160

120

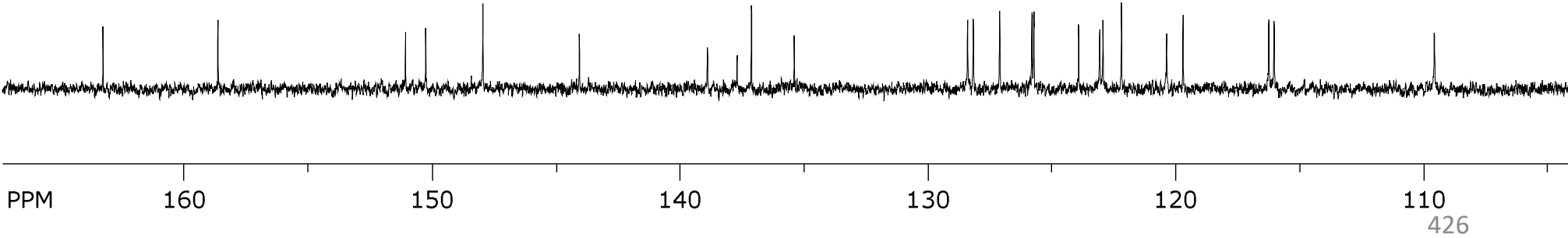
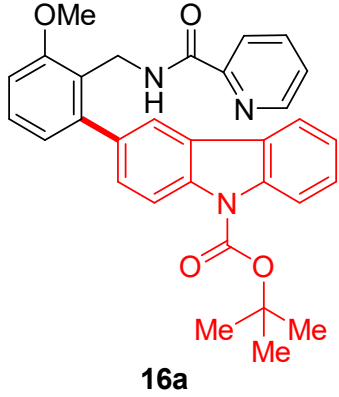
80

40

0

425

SpinWorks 4: RD-1169
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: RD 1177
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: RD 1177
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

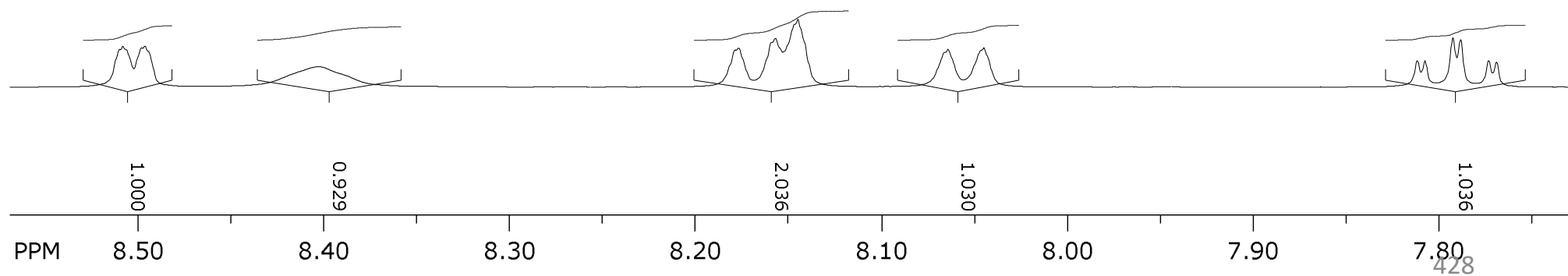
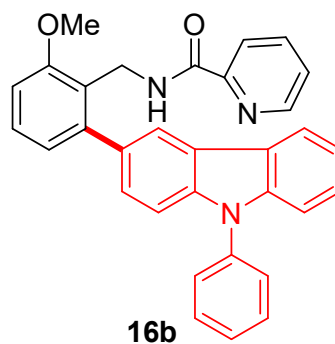
8.4967
8.4984
8.5069
8.5085
8.5102

8.4063

8.1449
8.1467
8.1570
8.1590
8.1768
8.1787

8.0448
8.0641

7.7686
7.7728
7.7879
7.7921
7.8071
7.8113



SpinWorks 4: RD 1177

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

7.6086
7.6196

7.4577
7.4701
7.4812
7.4920

7.4244

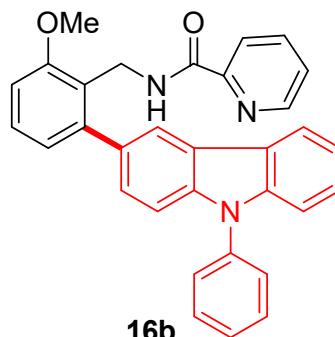
7.4059
7.4092

7.3850
7.3777
7.3748
7.3656
7.3589
7.3559
7.3469
7.3440

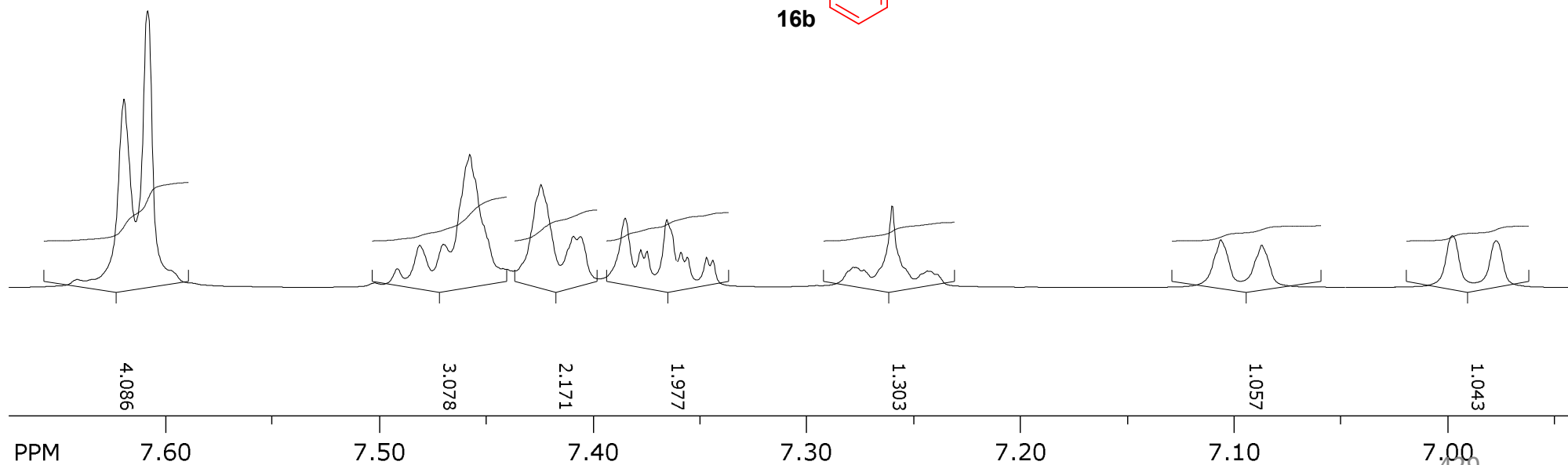
7.2788
7.2600
7.2467

7.1062
7.0870

6.9773
6.9977



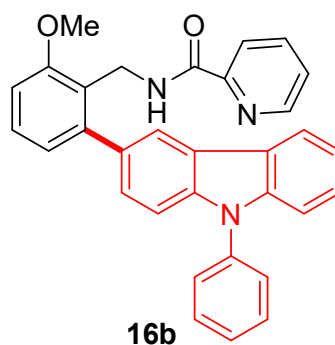
16b



SpinWorks 4: RD 1177
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

4.7282
4.7312
4.7414

3.9785



16b

2.008

3.071

PPM

4.8

4.6

4.4

4.2

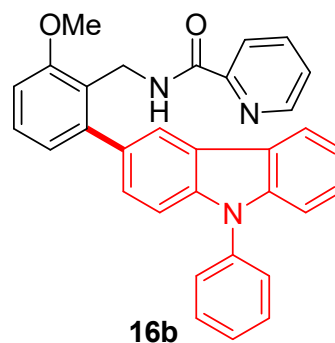
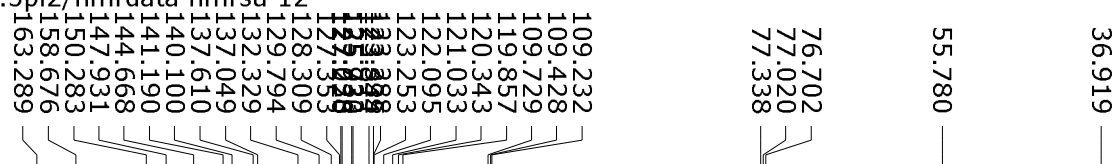
4.0

3.8

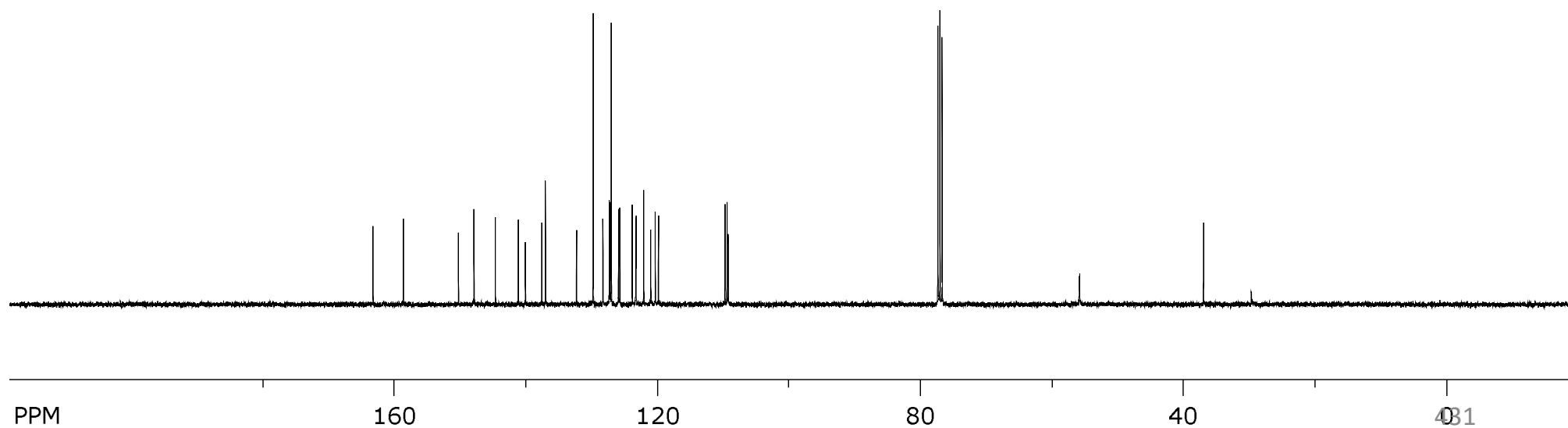
430

SpinWorks 4: RD 1177
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12



16b



SpinWorks 4: RD 1177

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

163.289

158.676

150.283

147.931

144.668

140.100

141.190

137.049

137.610

132.329

129.794

128.309

127.353

127.220

127.038

125.930

125.733

123.844

123.335

123.288

123.253

122.095

121.033

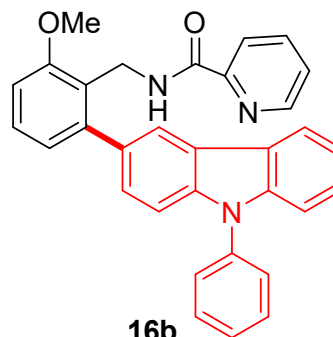
120.343

119.857

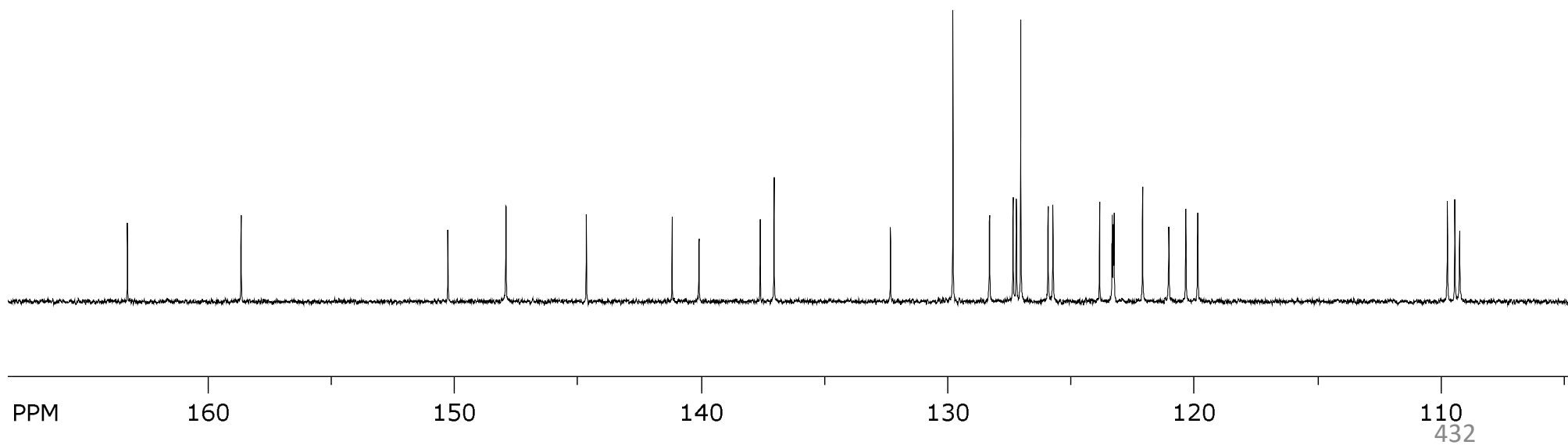
109.232

109.428

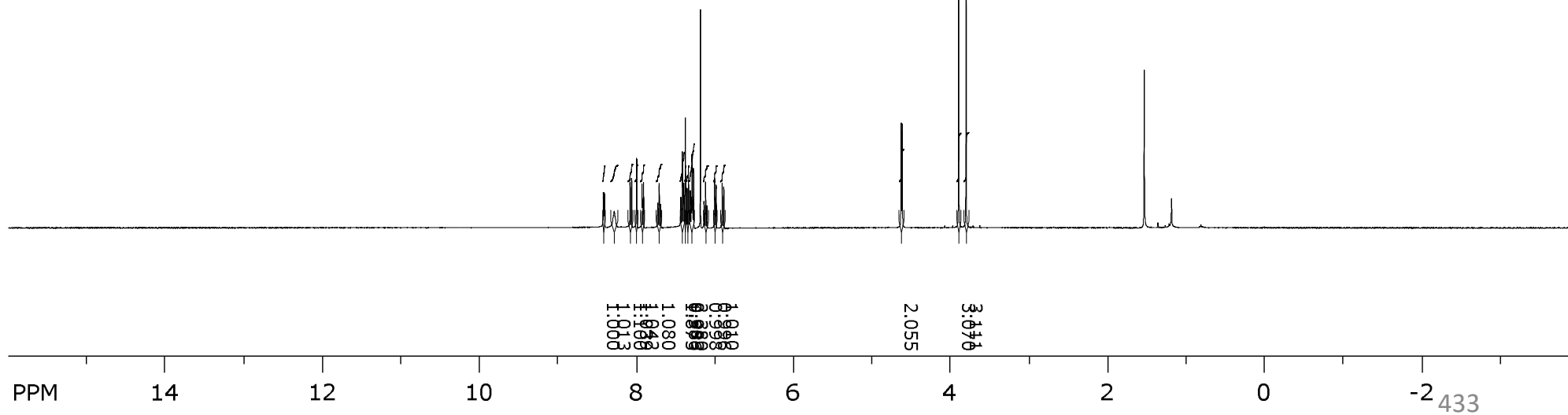
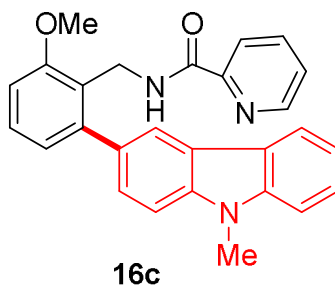
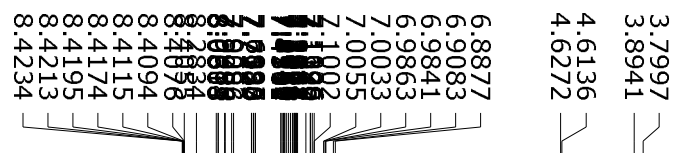
109.729



16b



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: RD-1180

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

8.4055
8.4076
8.4094
8.4115
8.4174
8.4195

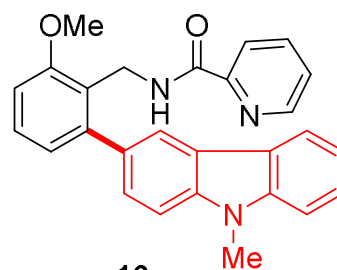
8.2834

8.0613
8.0634
8.0808

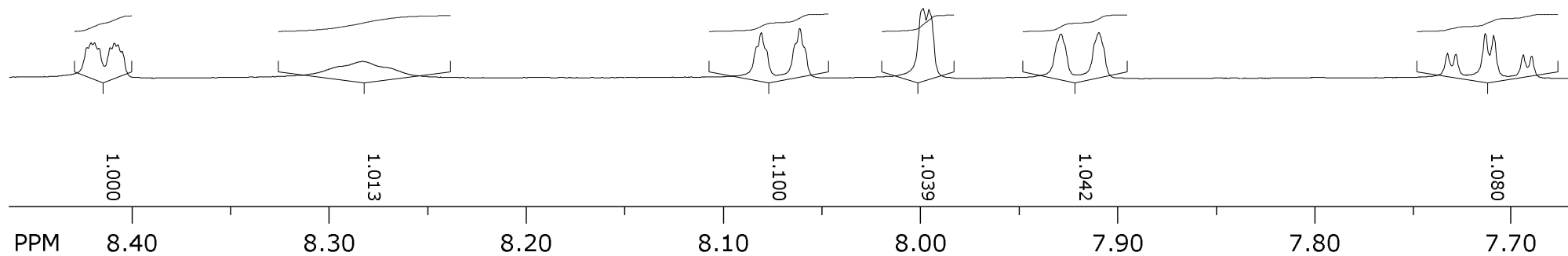
7.9957
7.9986

7.9093
7.9286

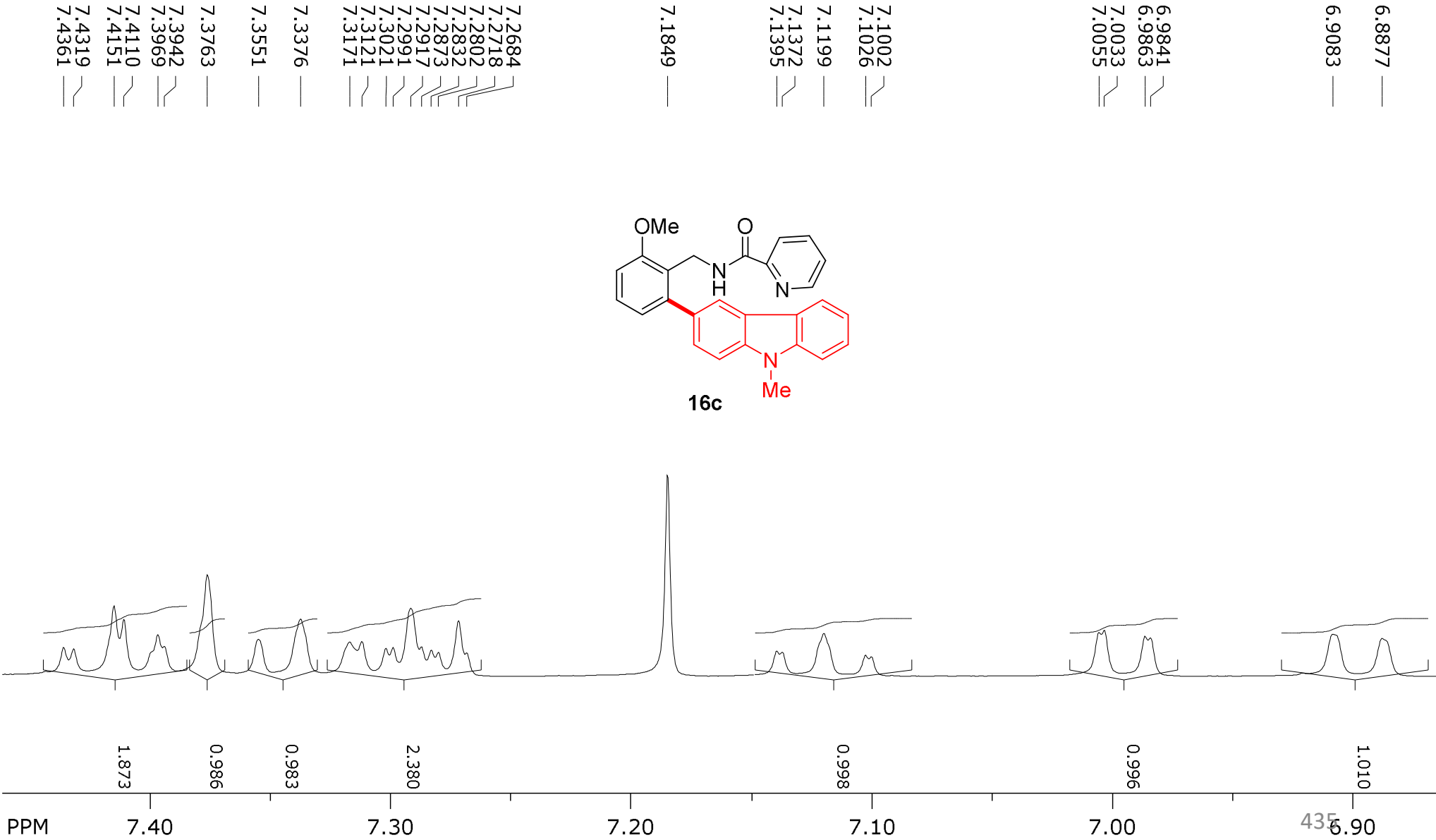
7.6995
7.6995
7.7088
7.7130
7.7280
7.7323



16c



SpinWorks 4: RD-1180
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

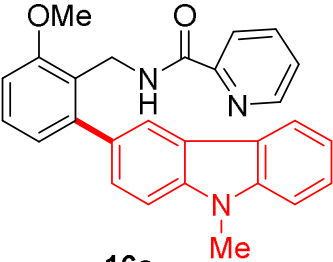


SpinWorks 4: RD-1180
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

4.6136
4.6272

3.8941

3.7997



16c

2.055

3.070

3.111

PPM 4.8 4.6 4.4 4.2 4.0 3.8 3.6

SpinWorks 4: RD-1180

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

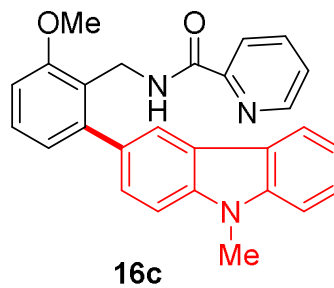
108.135
108.441
109.169
118.807
120.343
121.030
122.149
122.665
123.784
123.918
125.701
125.755
127.013
128.277
131.255
137.091
140.259
141.352
144.919
147.957
150.337
158.685
163.305

76.702
77.020
77.337

55.815

36.891

29.161



PPM

160

120

80

40

0

SpinWorks 4: RD-1180

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

163.305

158.685

150.337

147.957

144.919

140.259
141.352

137.091

131.255

128.277

127.013
125.755

125.701
123.918

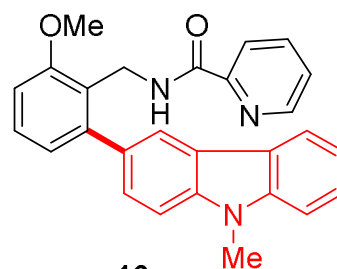
123.367
122.784

122.665
122.149

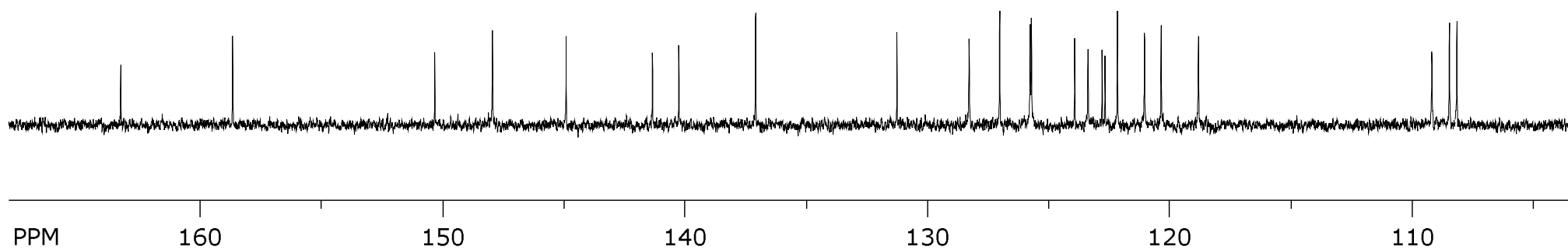
121.030
120.343

118.807

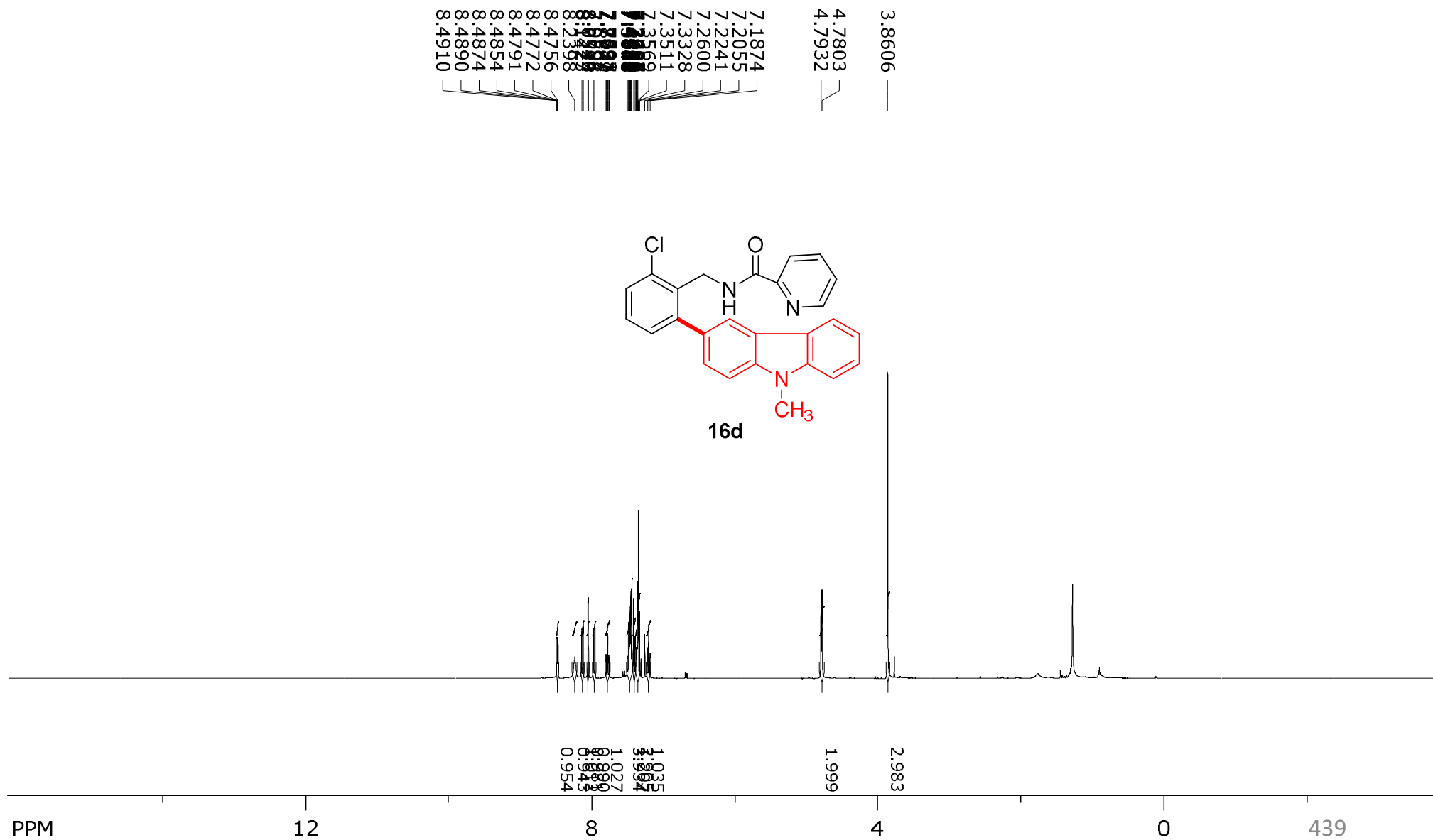
108.135
108.441
109.169



16c



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



SpinWorks 4: RD 1171

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 10

8.4756
8.4772
8.4791
8.4854
8.4874
8.4890

8.2398

8.1423

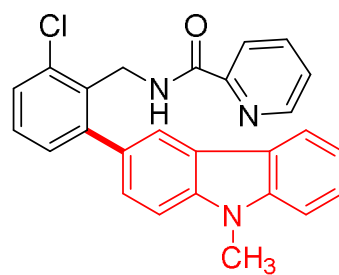
8.1227

8.0512
8.0529
8.0546

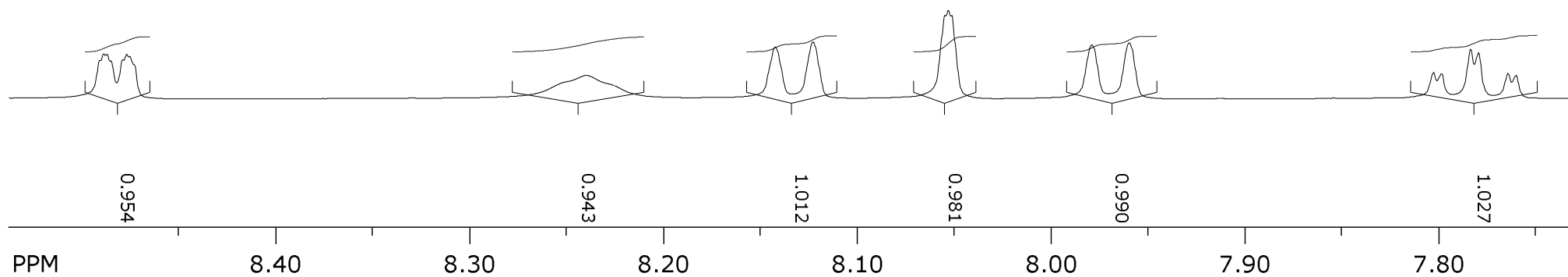
7.9788

7.9594

7.7597
7.7638
7.7791
7.7831
7.7982
7.8023



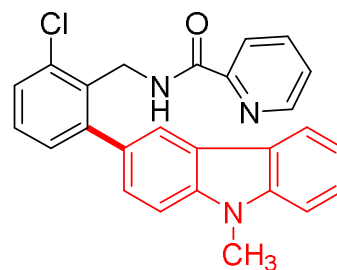
16d



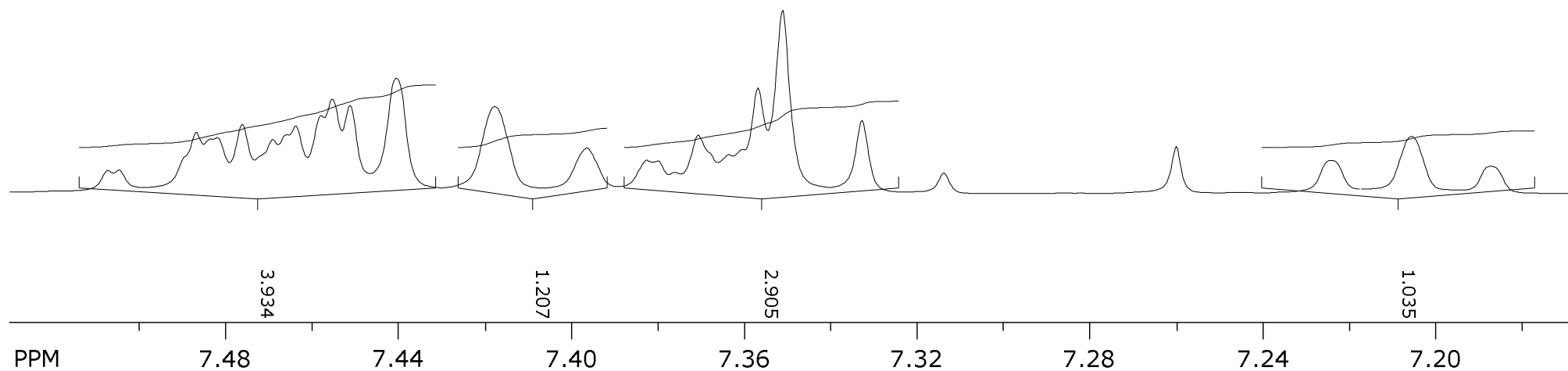
SpinWorks 4: RD 1171

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

7.5048	7.4406	7.4178	7.3965	7.3511	7.3328		7.2600		7.2241	7.2055	7.1874
7.5074	7.4513			7.3569							
	7.4554			7.3605							
	7.4580			7.3637							
	7.4639			7.3707							
	7.4661			7.3761							
	7.4693			7.3800							
	7.4763			7.3826							
	7.4821										
	7.4837										
	7.4869										



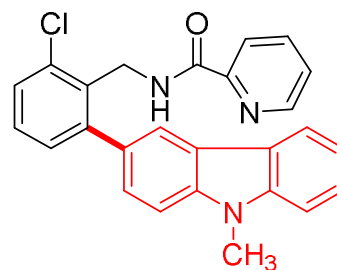
16d



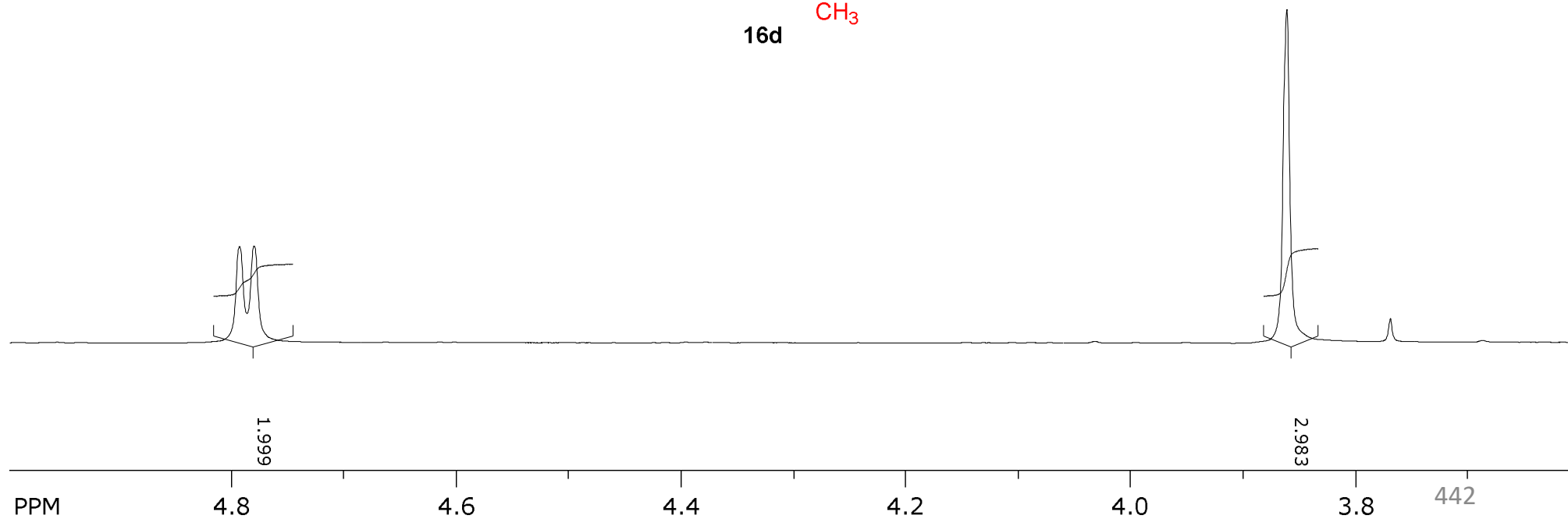
SpinWorks 4: RD 1171
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

4.7803
4.7932

3.8606



16d



SpinWorks 4: RD 1171

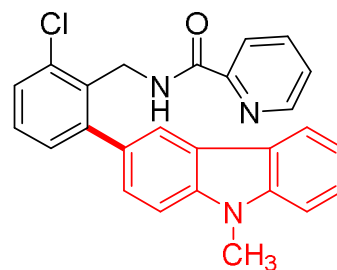
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

108.299
108.554
118.967
120.315
120.905
122.170
122.610
122.727
125.929
126.859
126.859
128.565
129.682
130.772
133.235
135.795
137.178
140.365
141.401
146.134
148.015
149.831
163.436

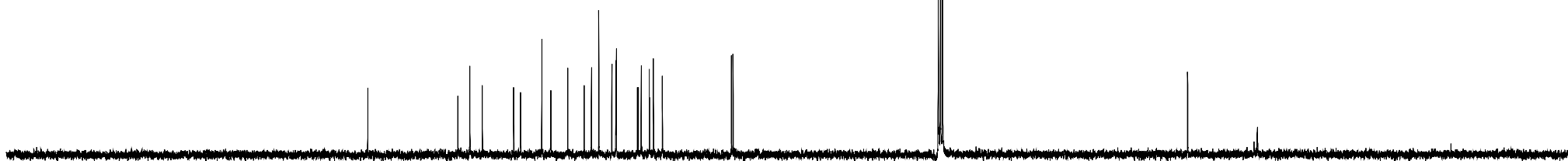
76.703
77.020
77.338

39.708

29.153



16d



PPM

160

120

80

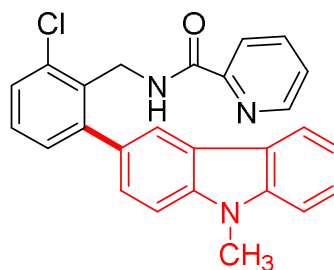
40

0
443

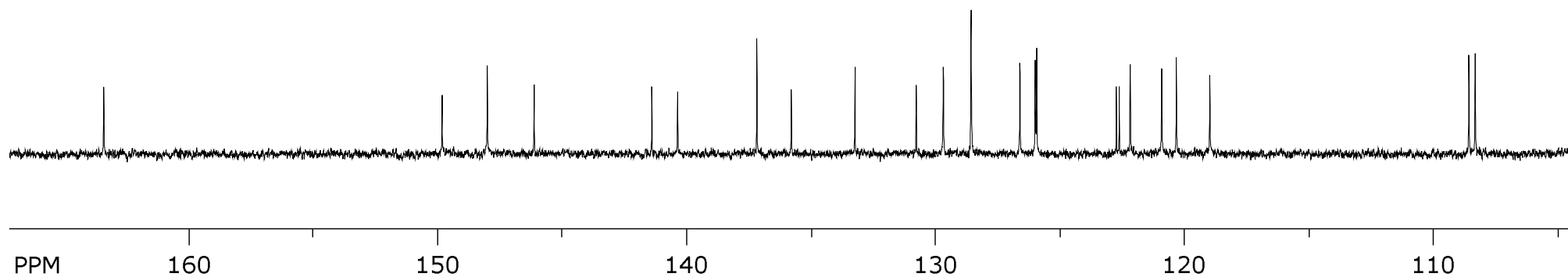
SpinWorks 4: RD 1171

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

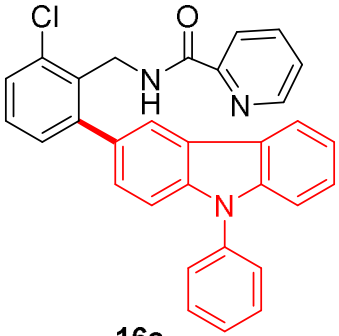
163.436	149.831	148.015	146.134	141.401	140.365	137.178	135.795	133.235	130.772	129.682	128.565	126.605	125.989	125.929	122.727	122.610	122.170	120.905	120.315	118.967	108.554	108.299
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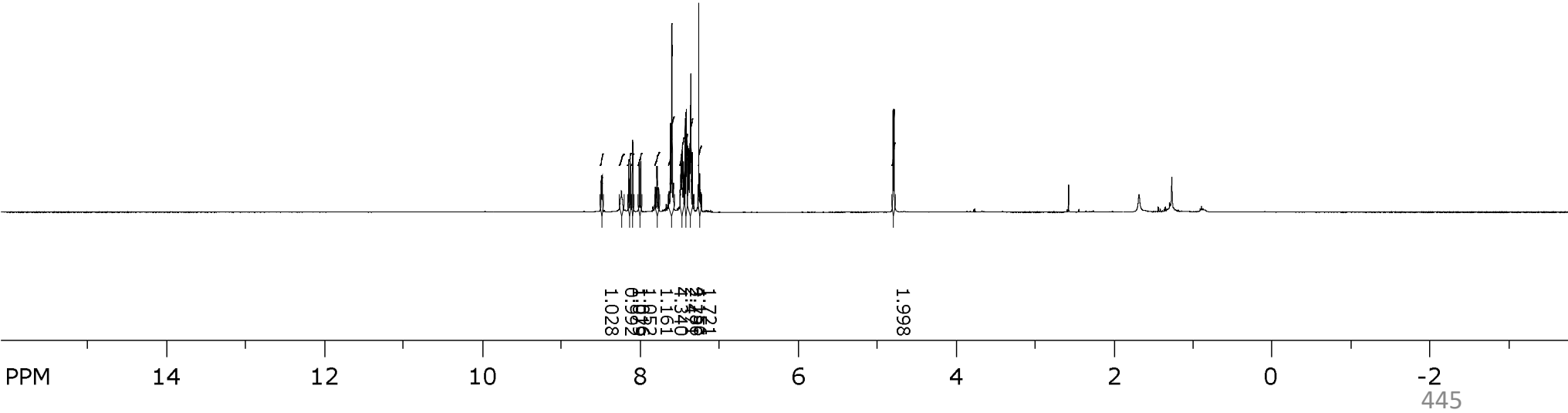
16d



SpinWorks 4: RD-1159
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 36



16e



SpinWorks 4: RD-1159
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 36

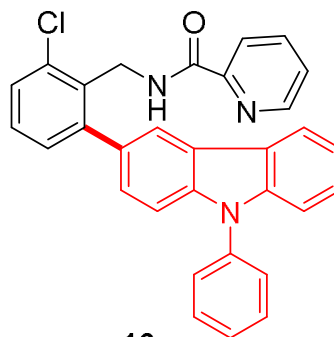
8.4795
8.4816
8.4834
8.4855
8.4914

8.2398

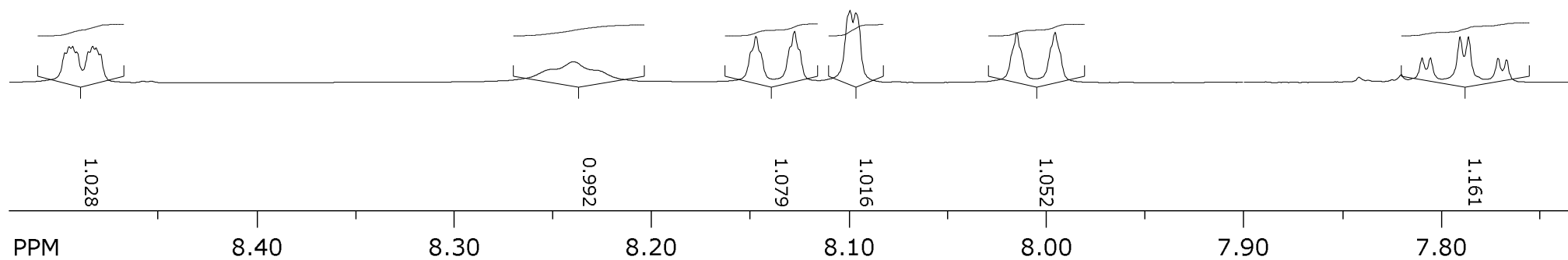
8.0965
8.0995
8.1276
8.1471

7.9955
8.0149

7.7667
7.7710
7.7860
7.7903
7.8053
7.8095

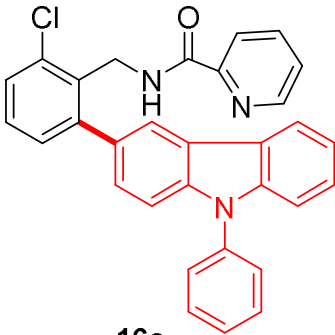


16e

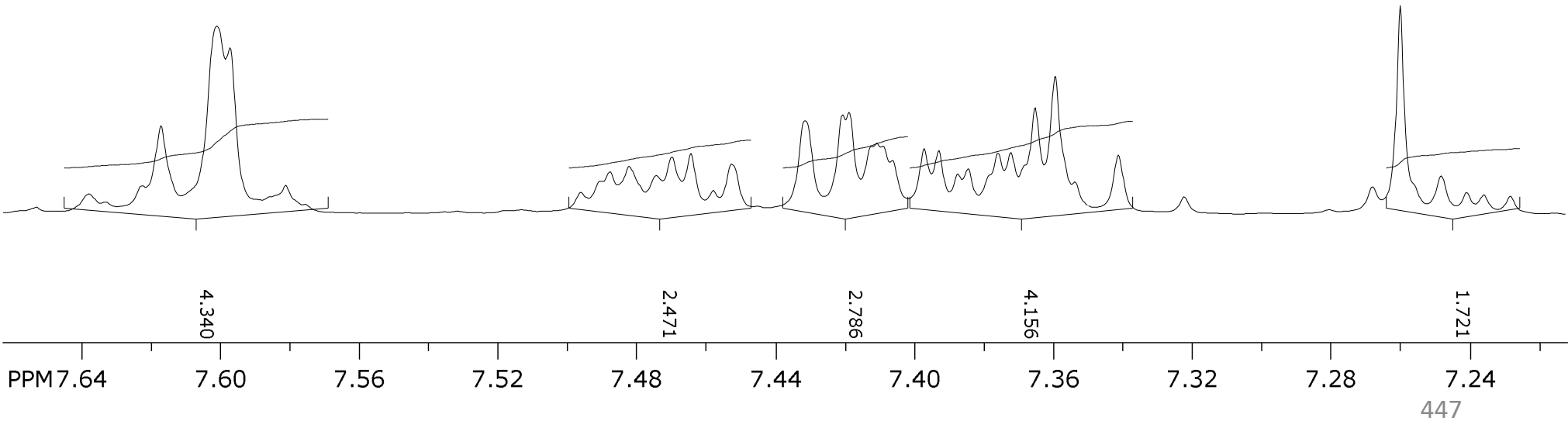


SpinWorks 4: RD-1159
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 36

7.6380	7.6011	7.4962	7.4316	7.2600
7.6332	7.5973	7.4905	7.4208	7.2482
7.6227	7.5898	7.4878	7.4189	7.2408
7.6172	7.5812	7.4823	7.4125	7.2360
		7.4745	7.4109	7.2283
		7.4700	7.4091	
		7.4645	7.4064	
		7.4580	7.3973	
		7.4528	7.3930	
			7.3875	
			7.3846	
			7.3759	
			7.3723	
			7.3652	
			7.3595	
			7.3538	
			7.3413	



16e



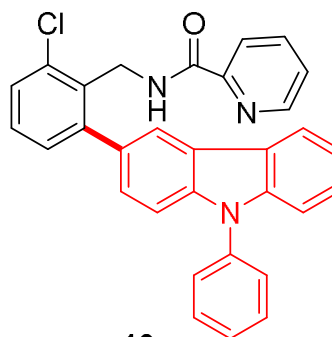
SpinWorks 4: RD 1159

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

109.602
109.836
119.985
120.296
120.882
122.129
123.128
123.302
125.979
129.898
131.827
131.827
133.146
135.811
137.154
137.463
140.218
141.257
145.906
147.984
149.763
163.419

76.703
77.020
77.338

39.733



16e

PPM

160

120

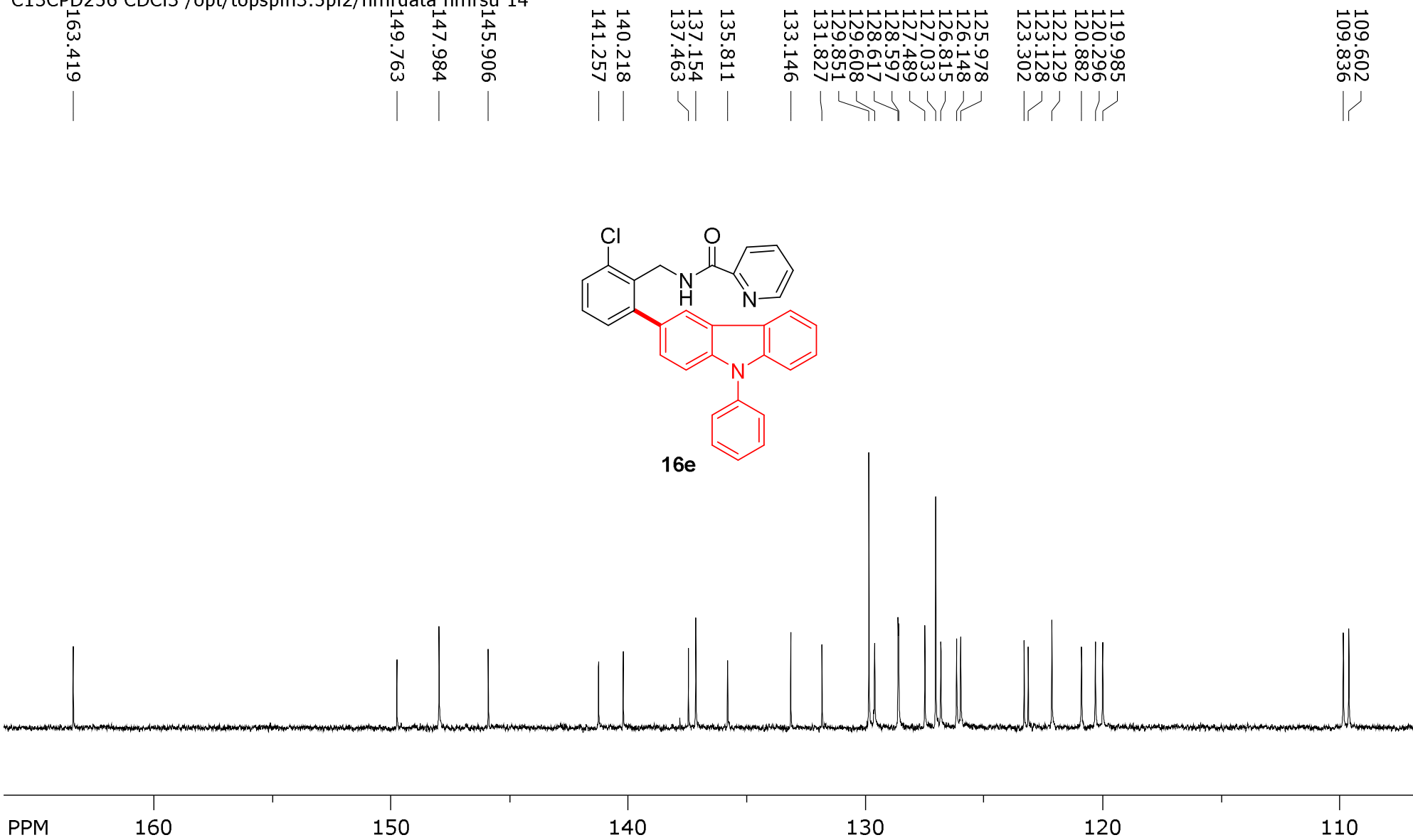
80

40

0

SpinWorks 4: RD 1159

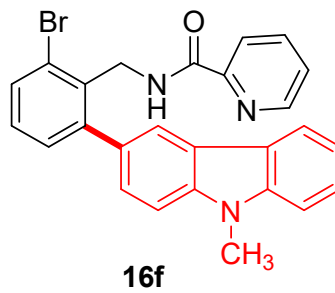
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14



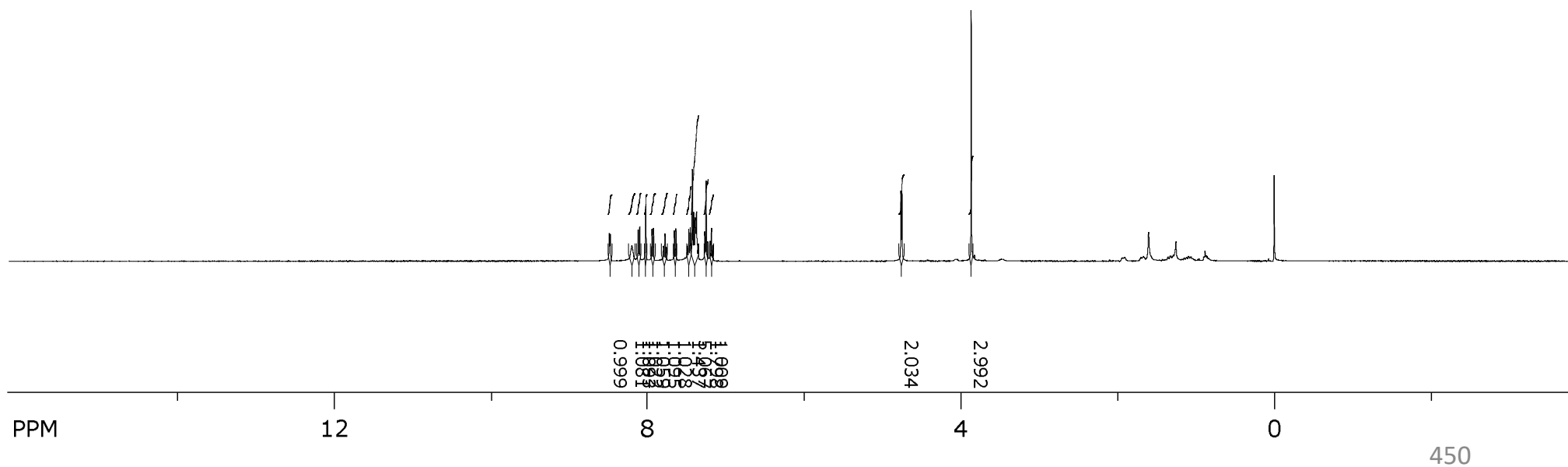
SpinWorks 4: RD 659

¹H

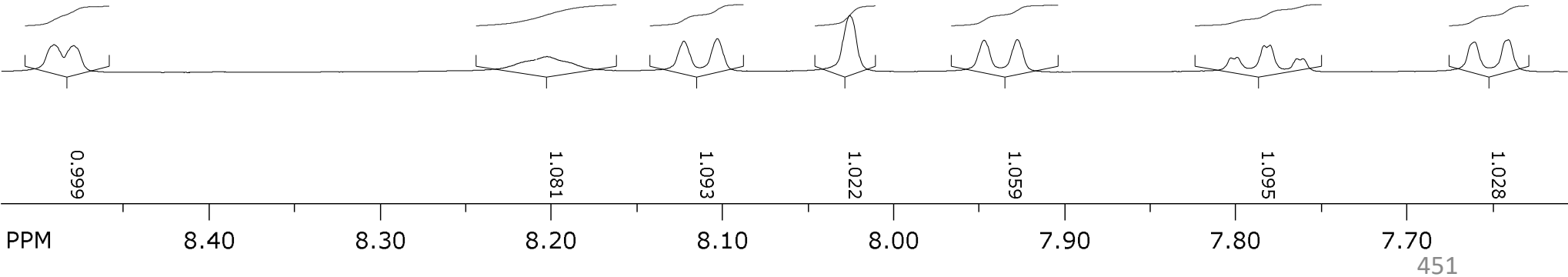
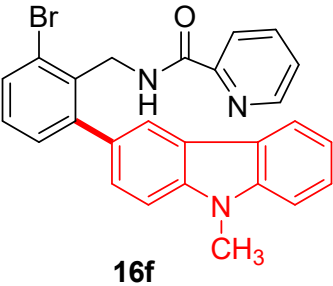
3.8697 —
4.7535 —
4.7664 —
7.1679 —
7.1866 —
7.2049 —
7.2330 —
7.2532 —
7.2572 —
7.2719 —
7.2899 —
7.2977 —
7.9277 —
7.9471 —
8.0256 —
8.1032 —
8.1227 —
8.2028 —
8.4793 —
8.4909 —



16f



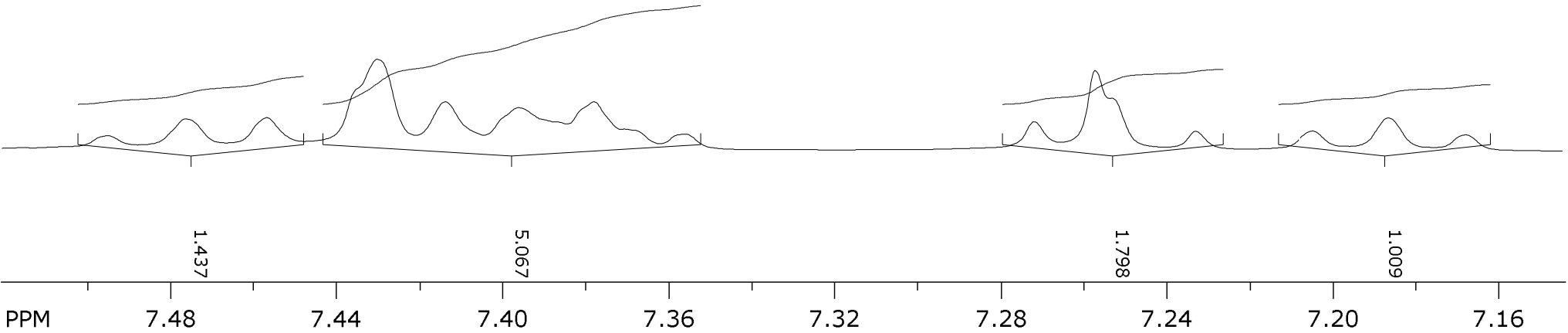
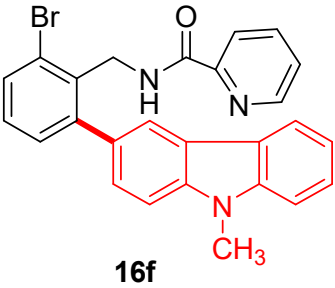
SpinWorks 4: RD 659



SpinWorks 4: RD 659

1H

7.4952	7.4764	7.4569	7.4302	7.4139	7.3962	7.3869	7.3780	7.3707	7.3561	7.2719	7.2532	7.2572	7.2330	7.2049	7.1866	7.1679
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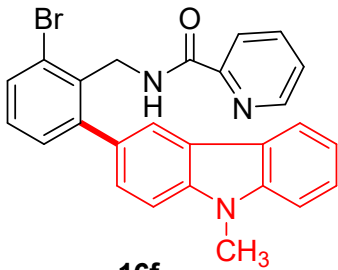


SpinWorks 4: RD 659

1H

4.7535
4.7664

3.8697



16f

2.034

2.992

PPM

4.8

4.6

4.4

4.2

4.0

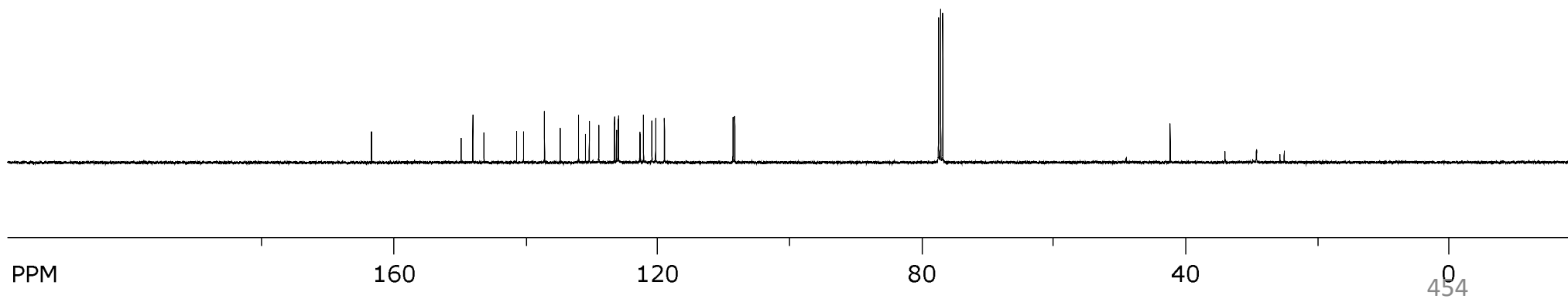
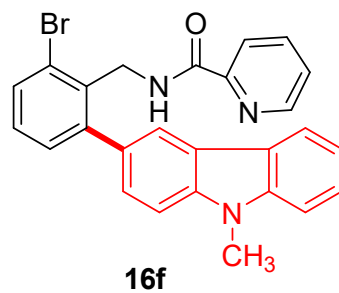
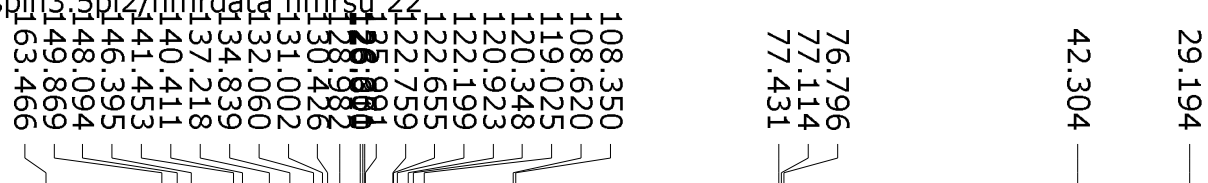
3.8

3.6

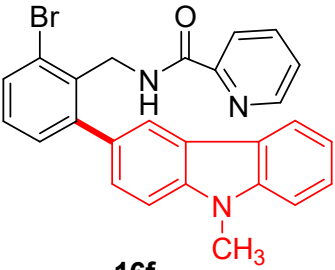
453

SpinWorks 4: RD-659

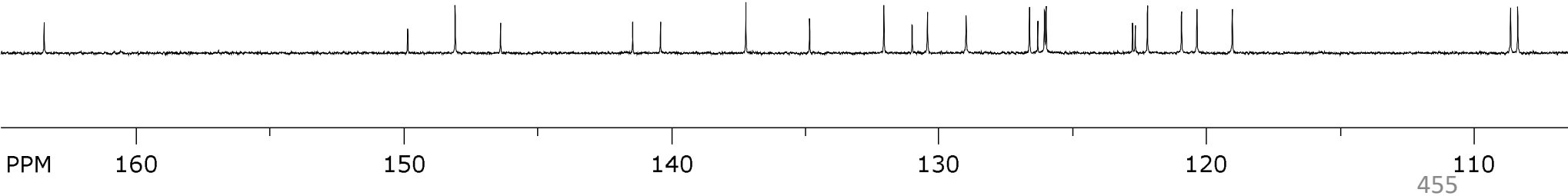
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu_22



SpinWorks 4: RD-659
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



16f



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 34



SpinWorks 4: RD-643

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 34

8.4927
8.5044

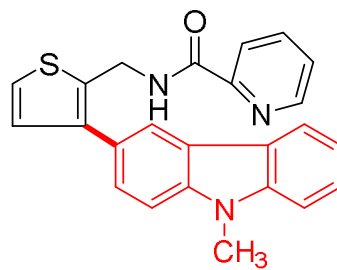
8.3858

8.2070
8.2265

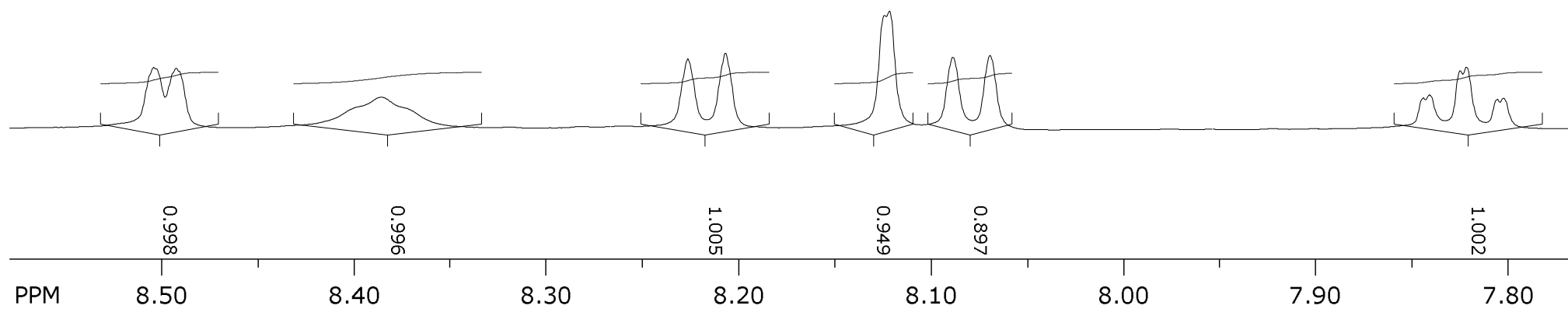
8.1216
8.1242

8.0693
8.0886

7.8022
7.8054
7.8215
7.8247
7.8406
7.8439

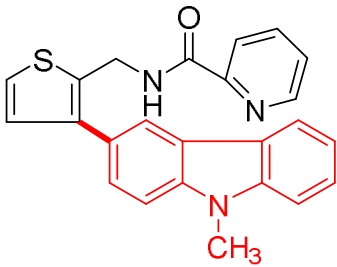


16g

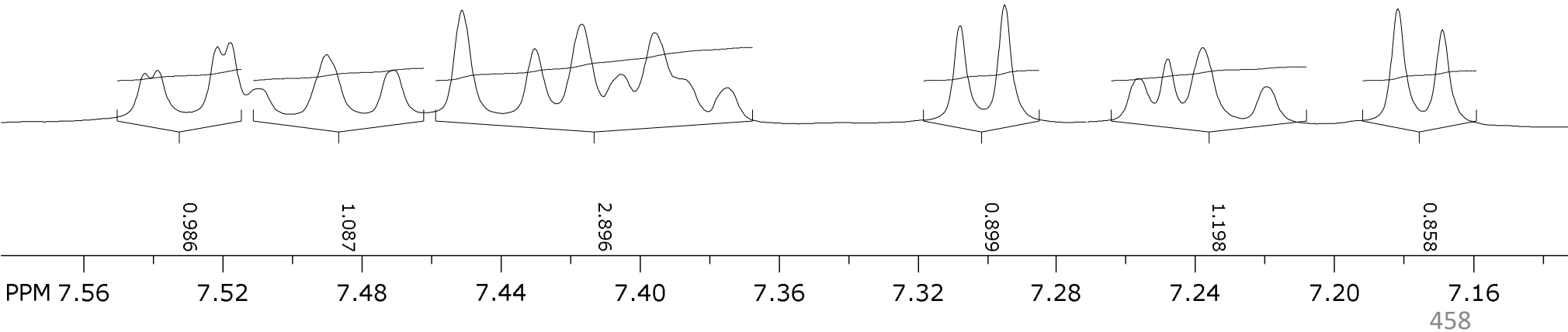


SpinWorks 4: RD-643
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 34

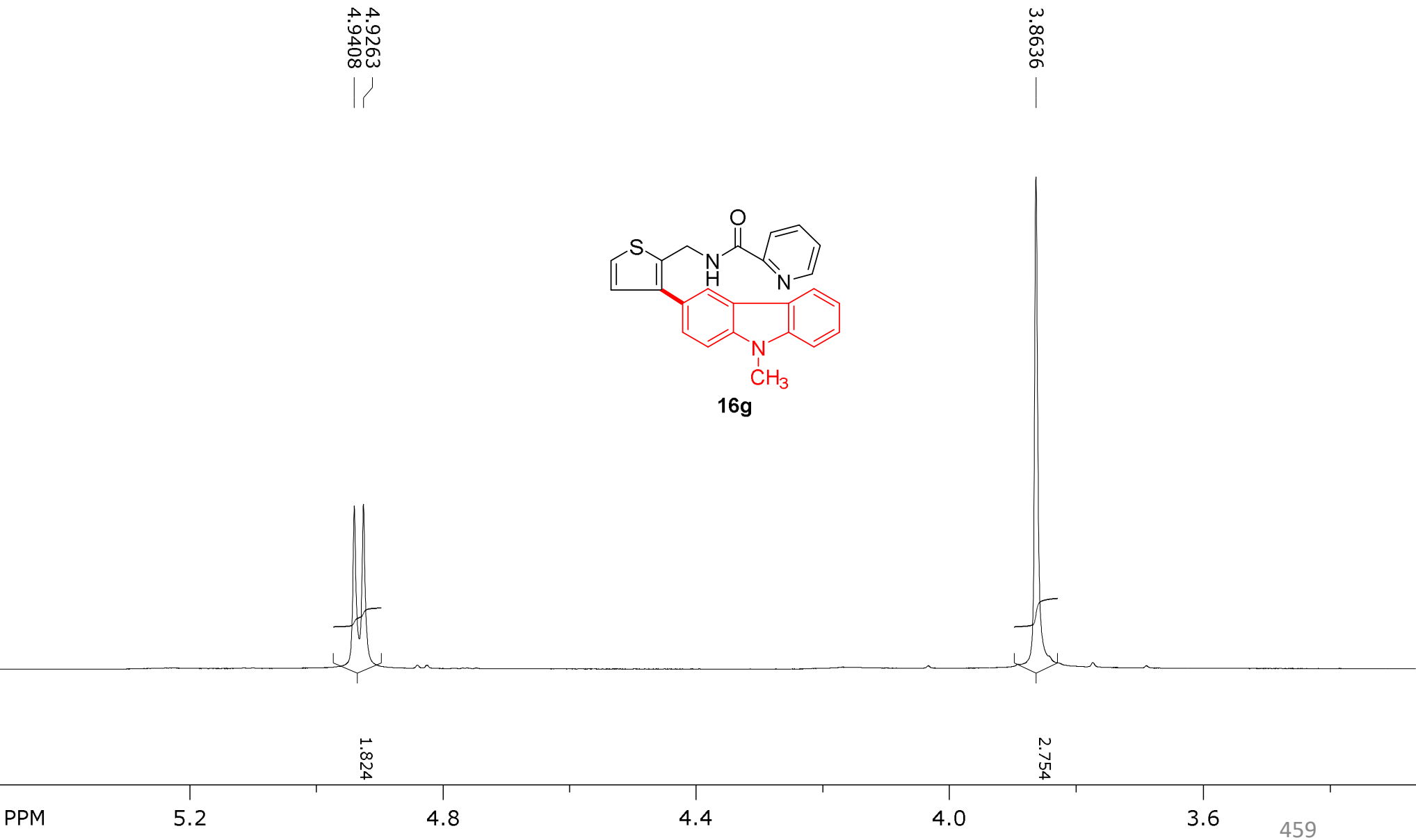
7.1689	—
7.1817	—
7.2194	—
7.2379	—
7.2479	—
7.2562	—
7.2950	—
7.3078	—
7.3749	—
7.3877	—
7.3958	—
7.4056	—
7.4168	—
7.4303	—
7.4513	—
7.4709	—
7.4903	—
7.5093	—
7.5105	—
7.5180	—
7.5217	—
7.5390	—
7.5426	—



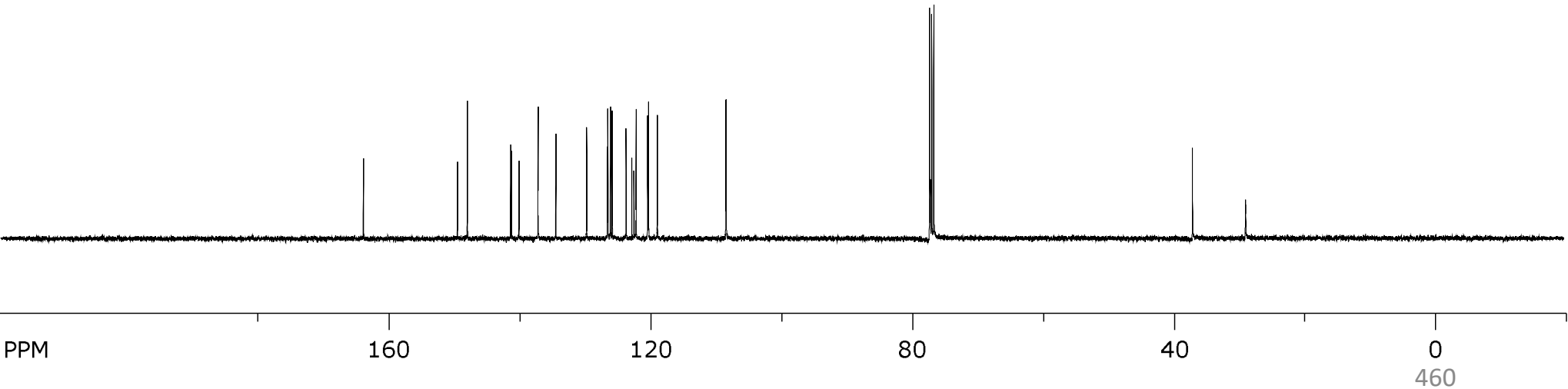
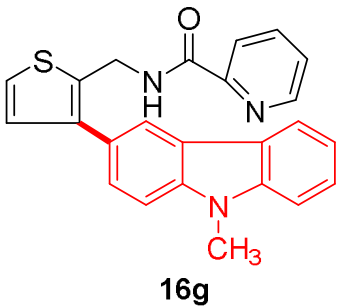
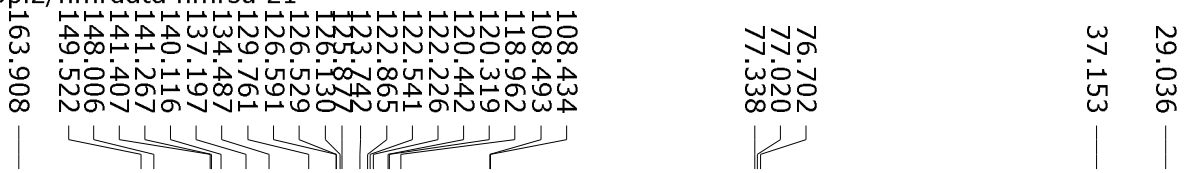
16g



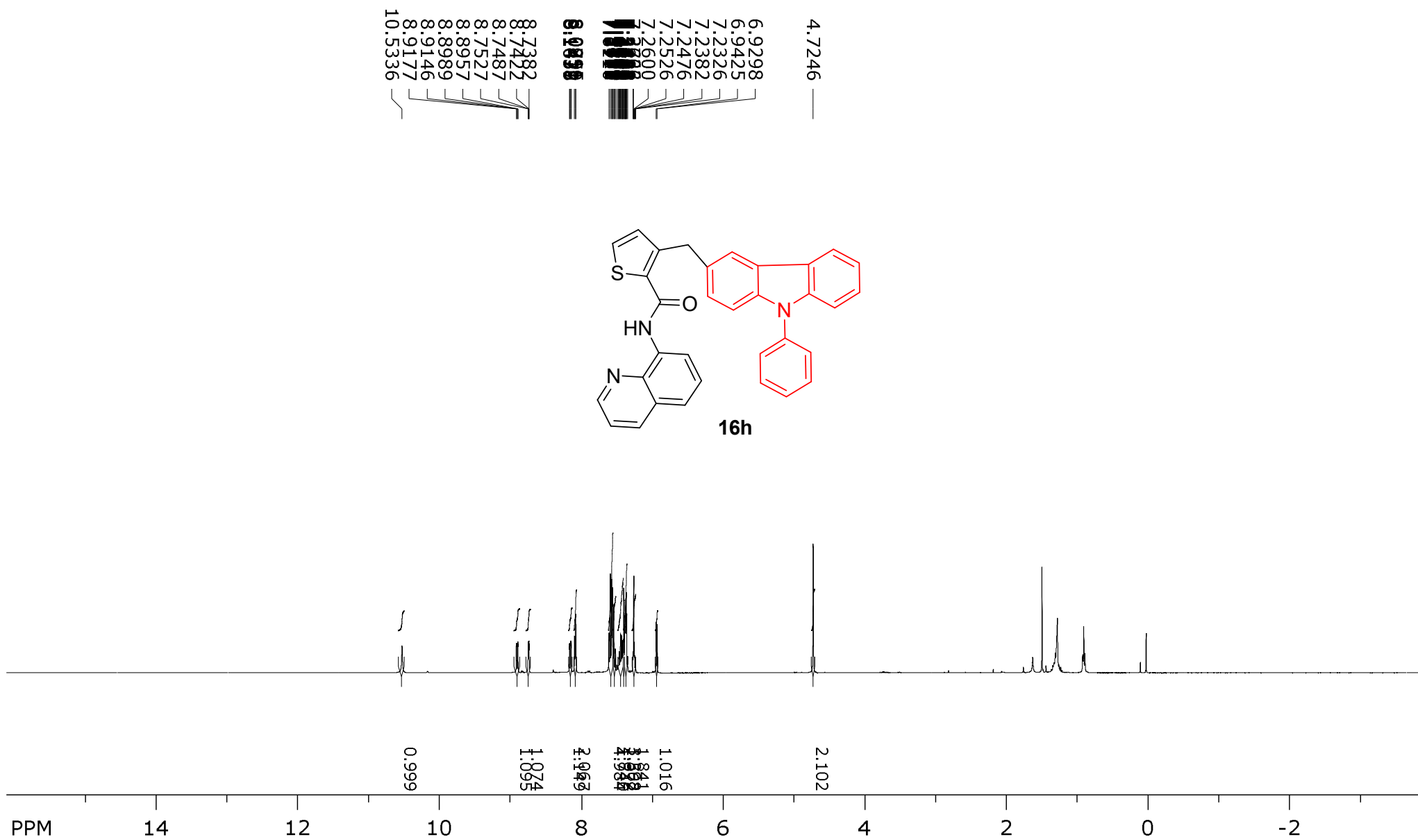
SpinWorks 4: RD-643
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 34



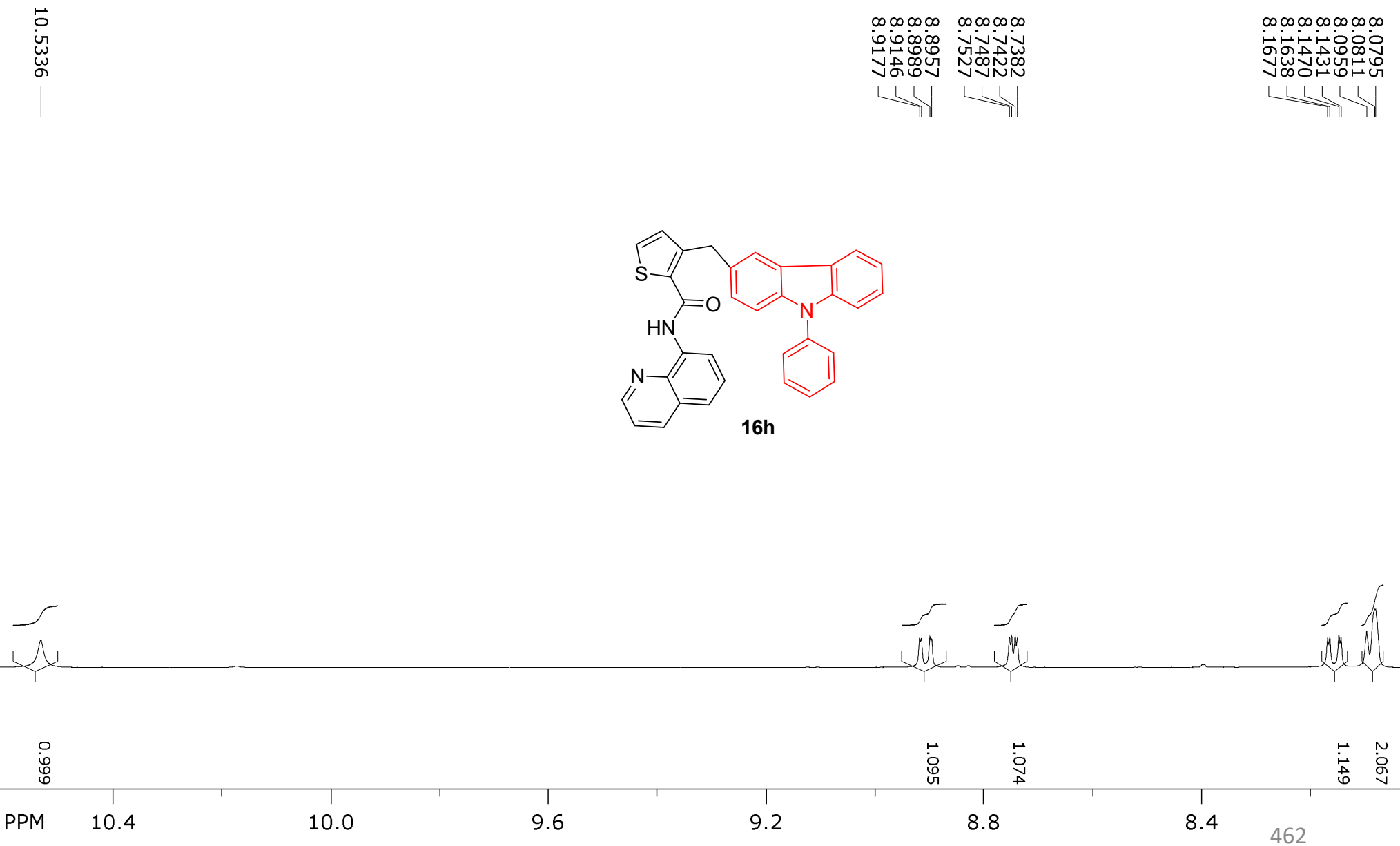
SpinWorks 4: RD-643
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



SpinWorks 4: rd-336a



SpinWorks 4: rd-336a



SpinWorks 4: rd-336a

7.2326
7.2382
7.2476
7.2526
7.2600
7.2666
7.2723

7.3460
7.3606
7.3667
7.3732
7.3767
7.3808
7.3840
7.3869

7.4015
7.4115
7.4160
7.4179
7.4220
7.4320

7.4428
7.4478

7.4613
7.4655
7.4694
7.4792

7.4964
7.4992

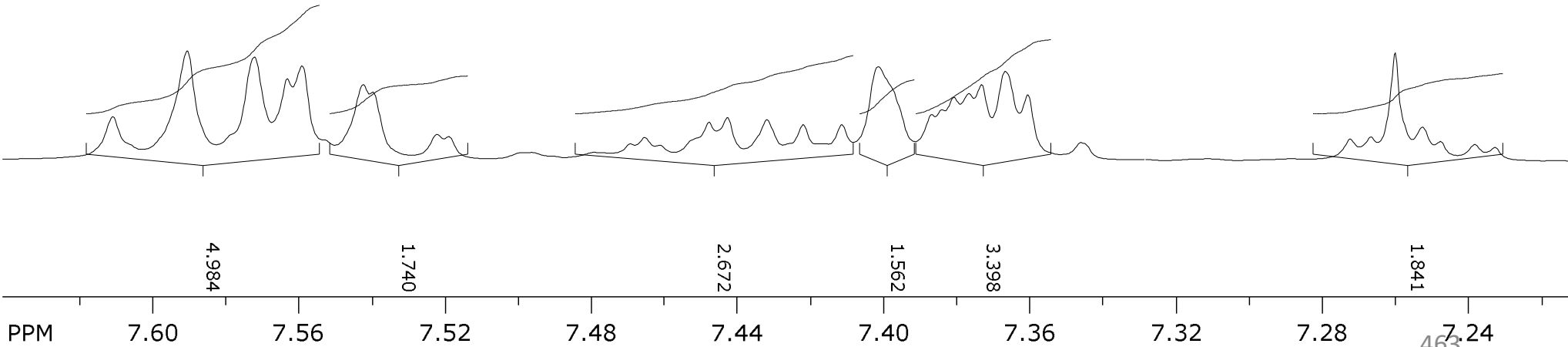
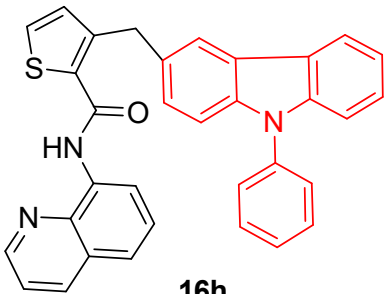
7.5191
7.5223

7.5399
7.5425

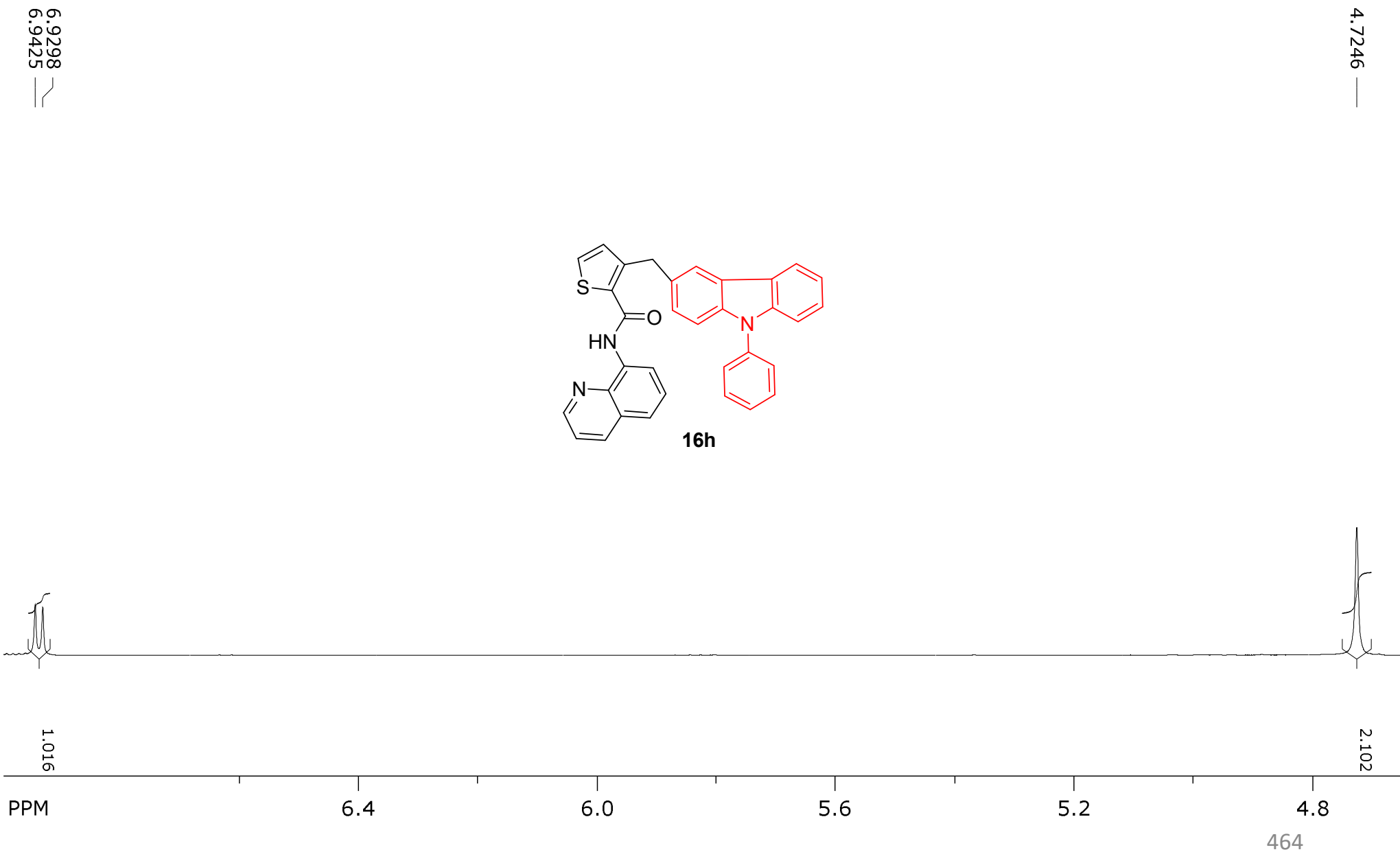
7.5592
7.5633
7.5722

7.5907

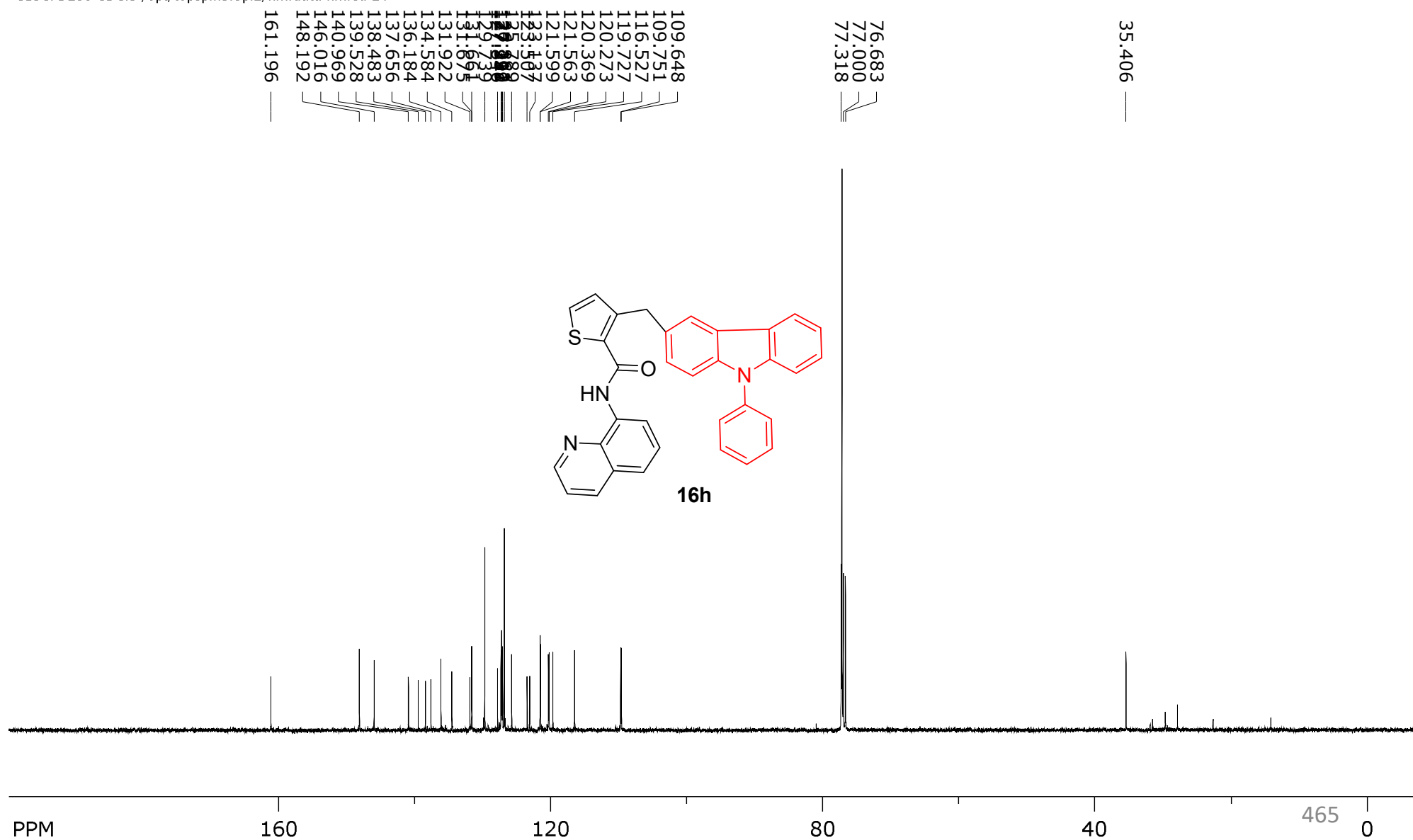
7.6110



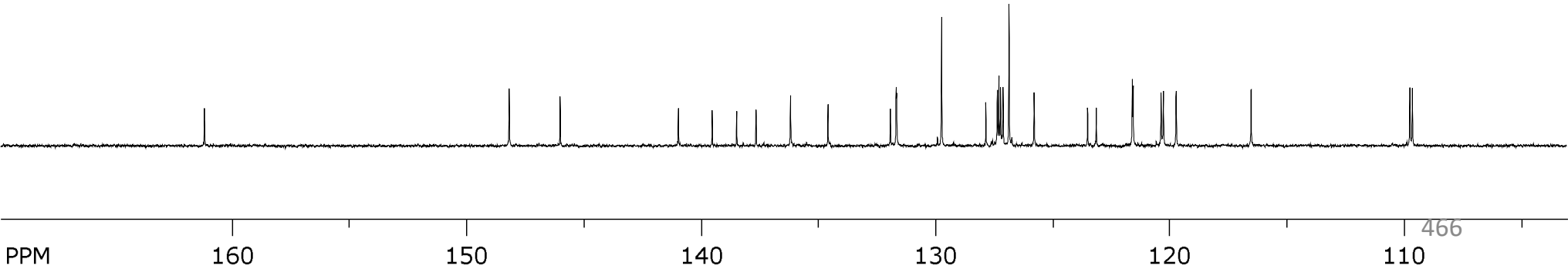
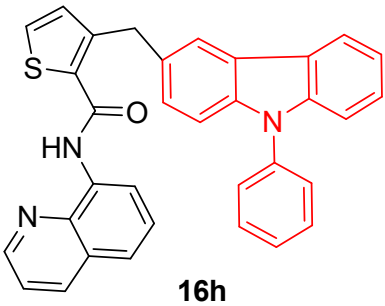
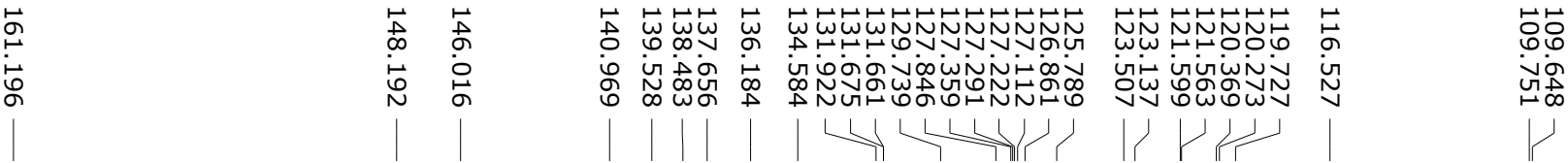
SpinWorks 4: rd-336a



SpinWorks 4: RD 336 A
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



SpinWorks 4: RD 336 A
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24



SpinWorks 4: RD-713
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

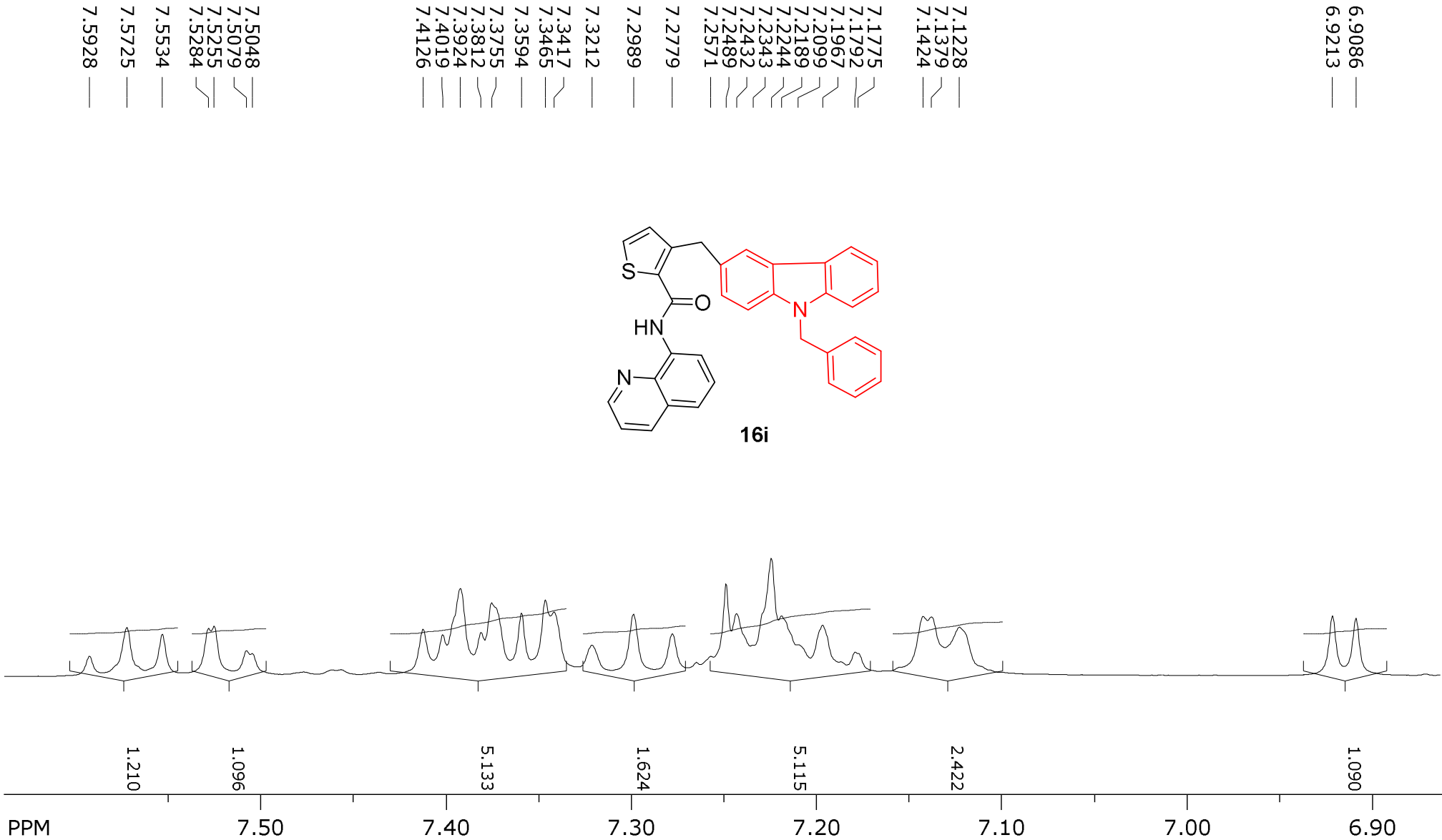


SpinWorks 4: RD-713

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33



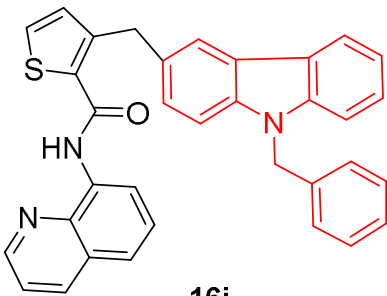
SpinWorks 4: RD-713
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33



SpinWorks 4: RD-713
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

5.4766

4.6898



16i

2.297

2.128

PPM 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4

SpinWorks 4: RD-713

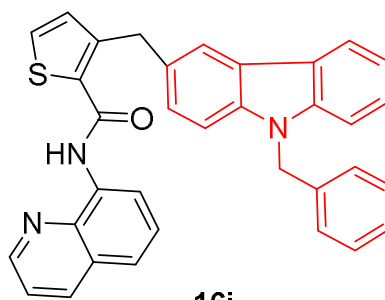
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

161.262
148.235
145.923
140.876
139.404
138.552
137.205
136.217
134.658
132.137
131.754
130.933
129.718
128.895
128.895
121.627
121.600
120.497
120.401
119.038
116.592
108.904
108.819

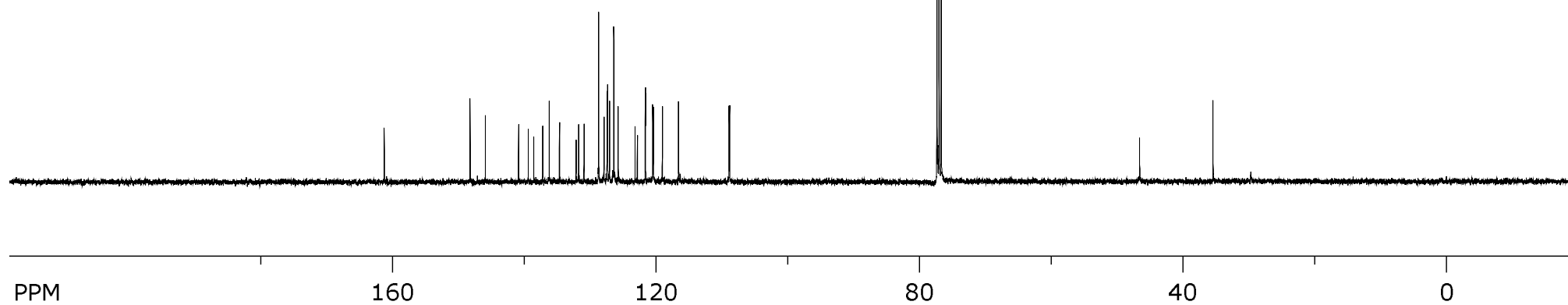
76.702
77.020
77.338

46.558

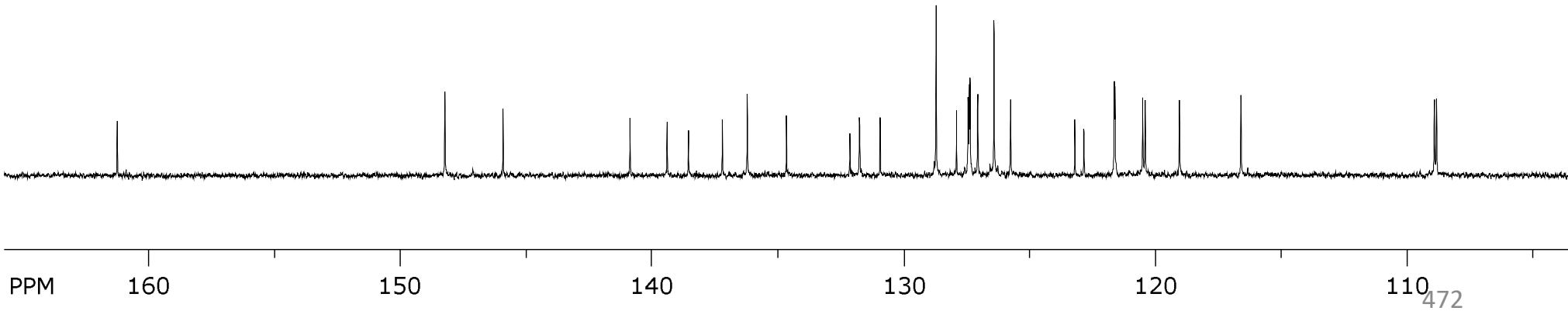
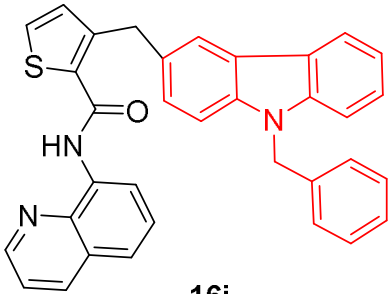
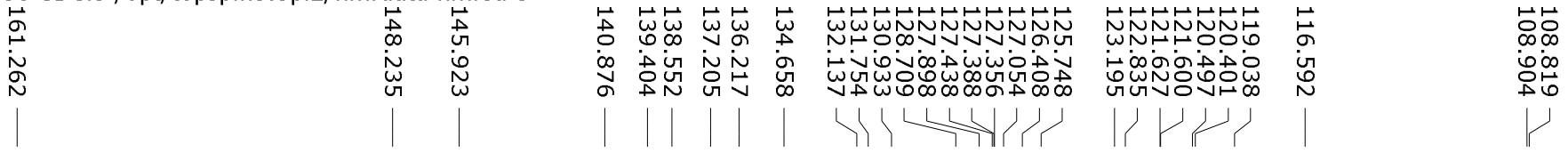
35.422



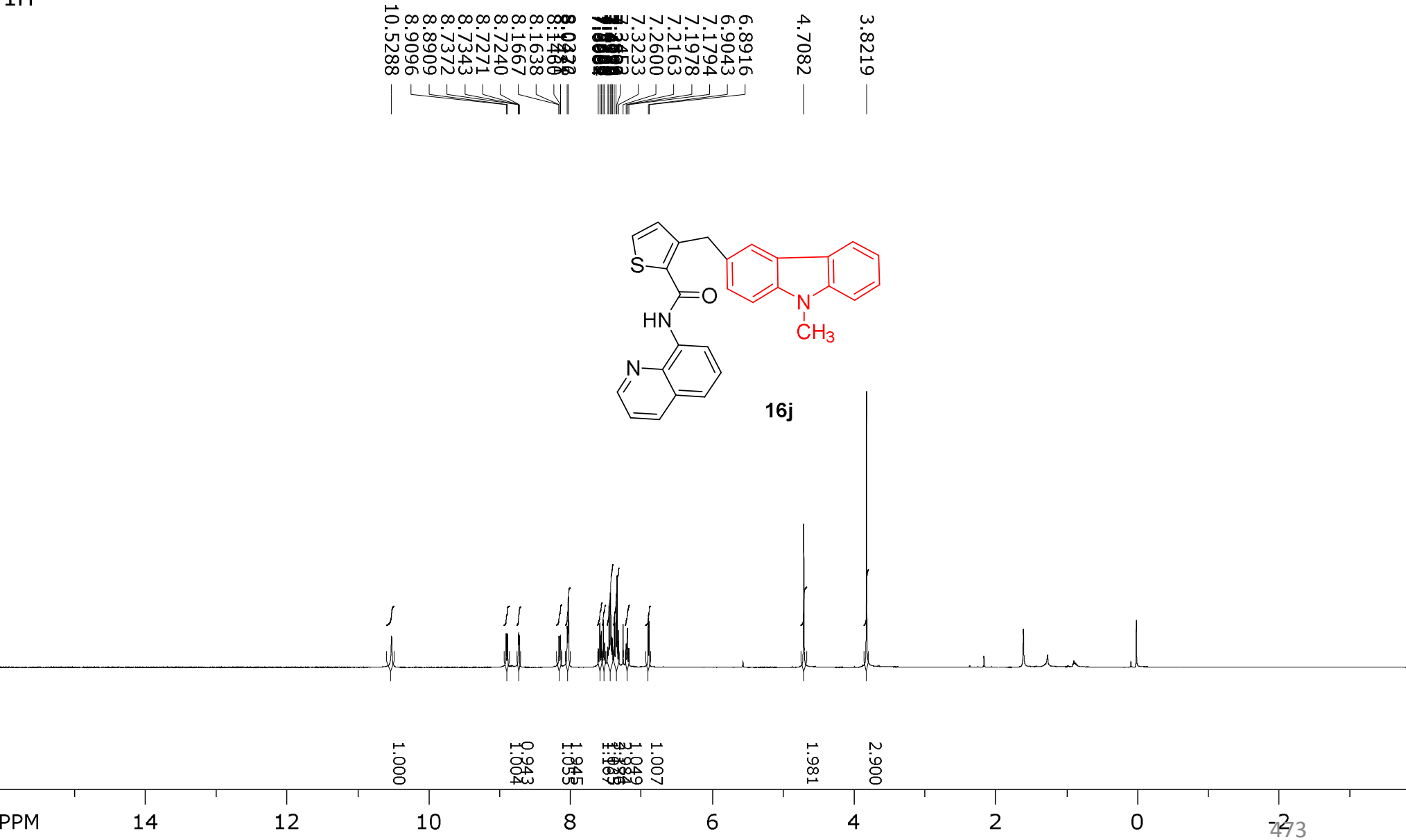
16i



SpinWorks 4: RD-713
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: RD 641
1H



SpinWorks 4: RD 641

¹H

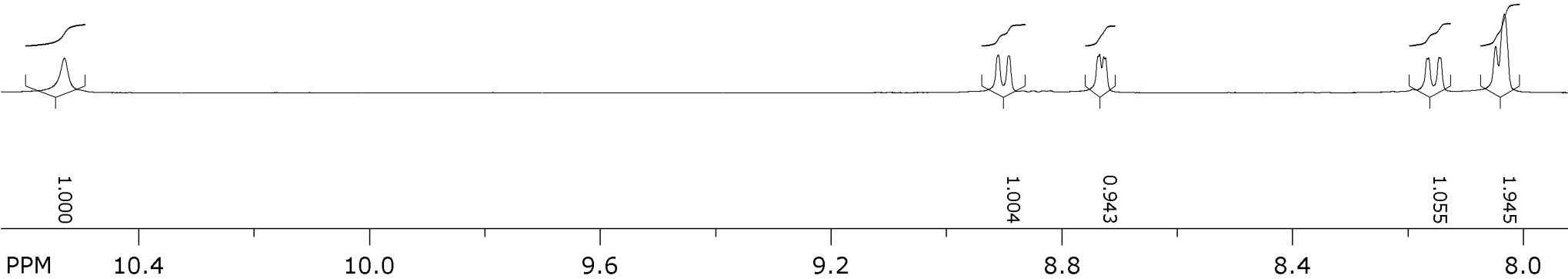
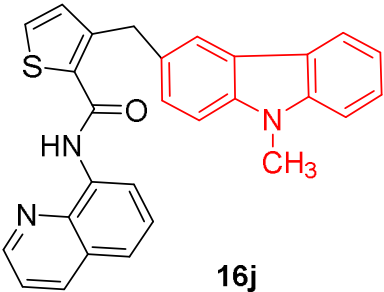
10.5288

8.7240
8.7271
8.7343
8.7372

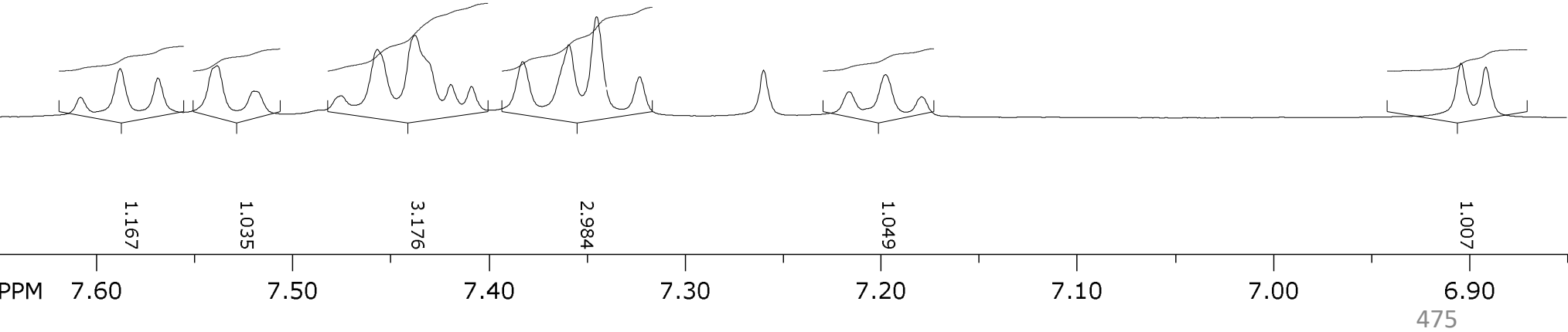
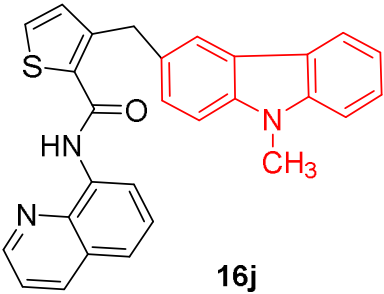
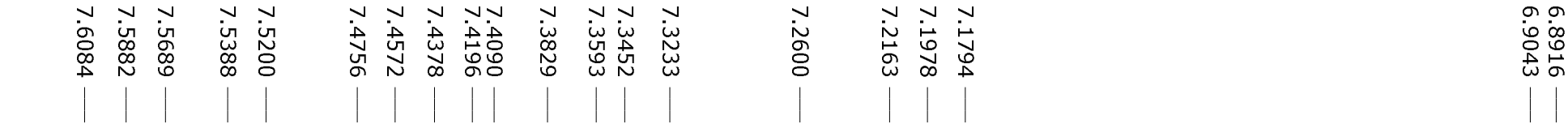
8.8909
8.9096

8.1431
8.1460
8.1638
8.1667

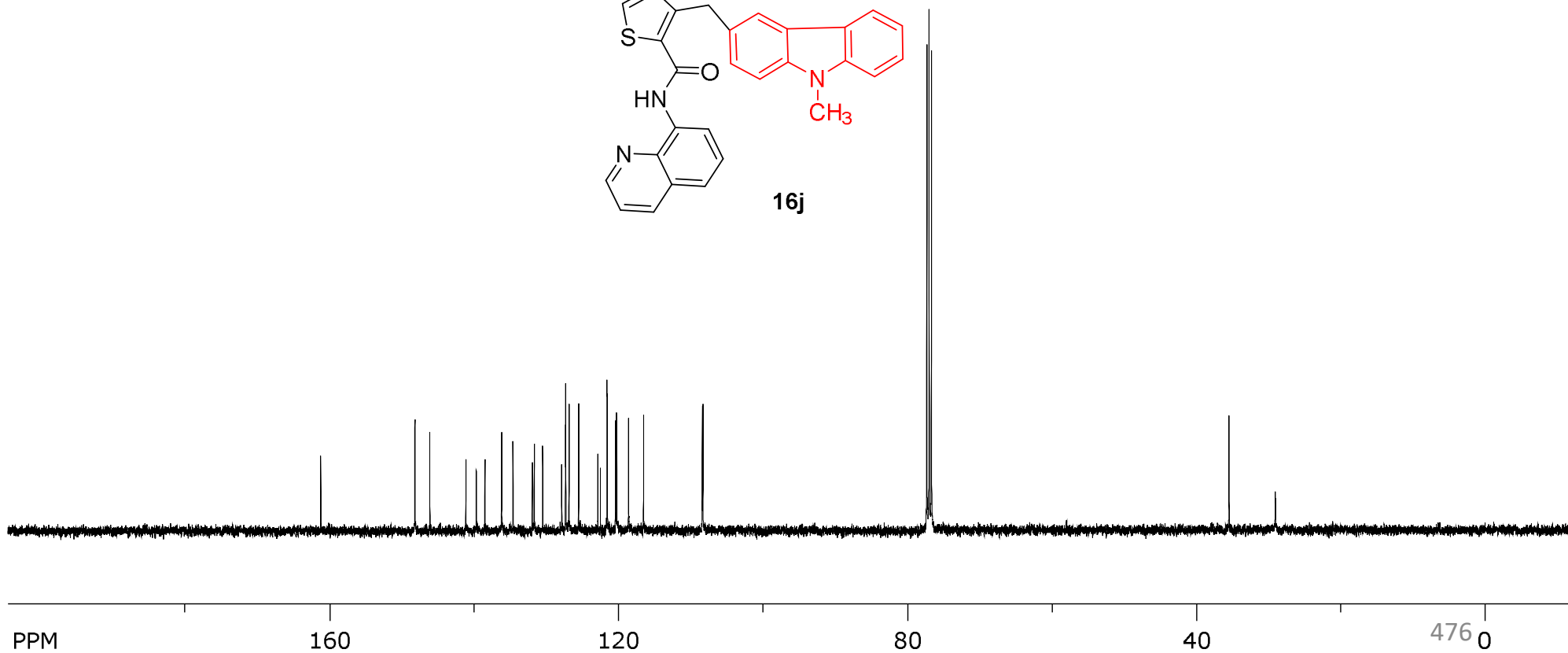
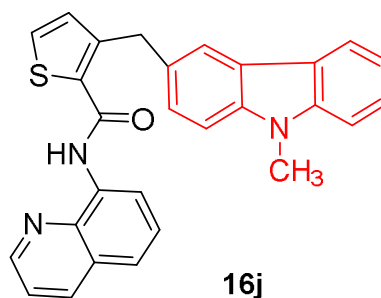
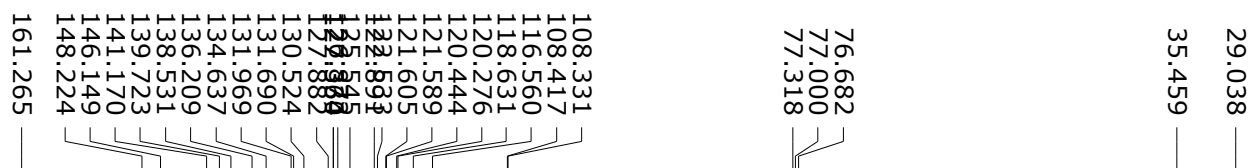
8.0322
8.0476



SpinWorks 4: RD 641
1H

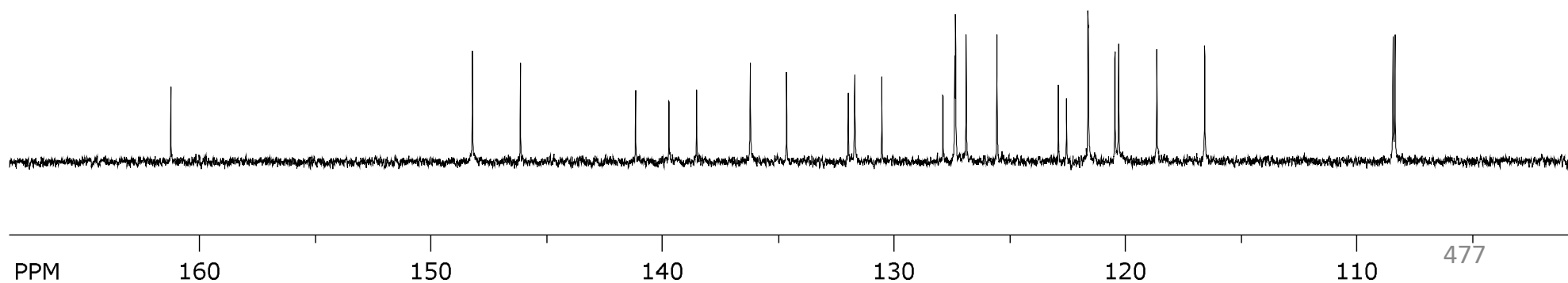
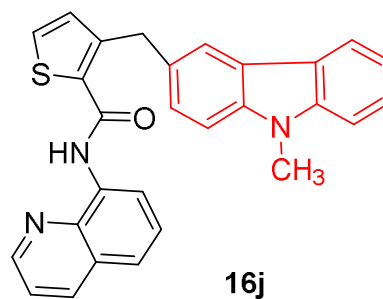


SpinWorks 4: RD-641
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

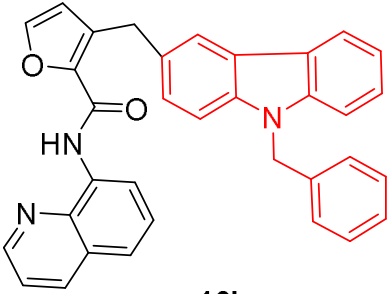


SpinWorks 4: RD-641
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

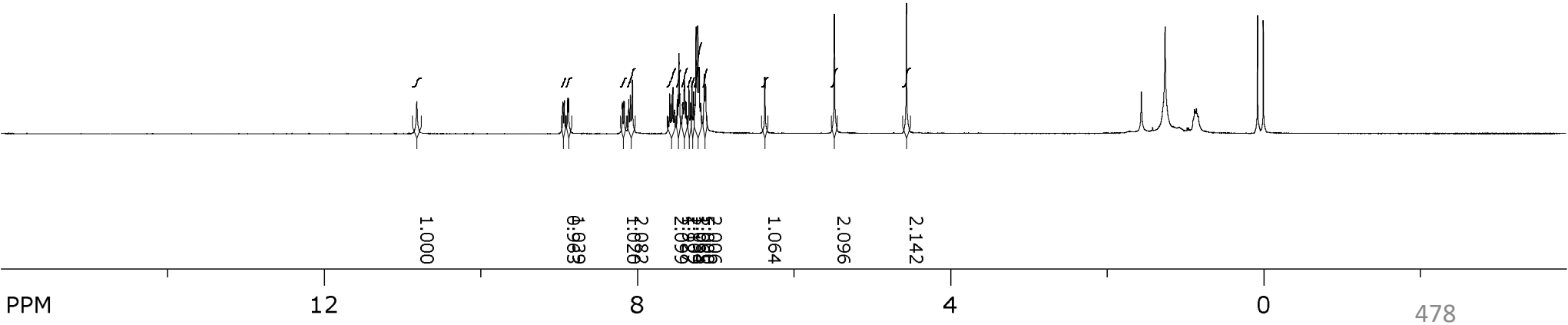
108.331	116.560	125.545	127.882	130.524	131.690	131.969	134.637	136.209	138.531	139.723	141.170	146.149	148.224	161.265
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



SpinWorks 4: RD-715Re
1H



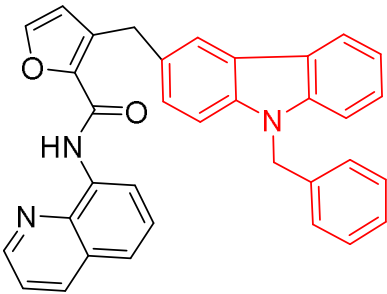
16k



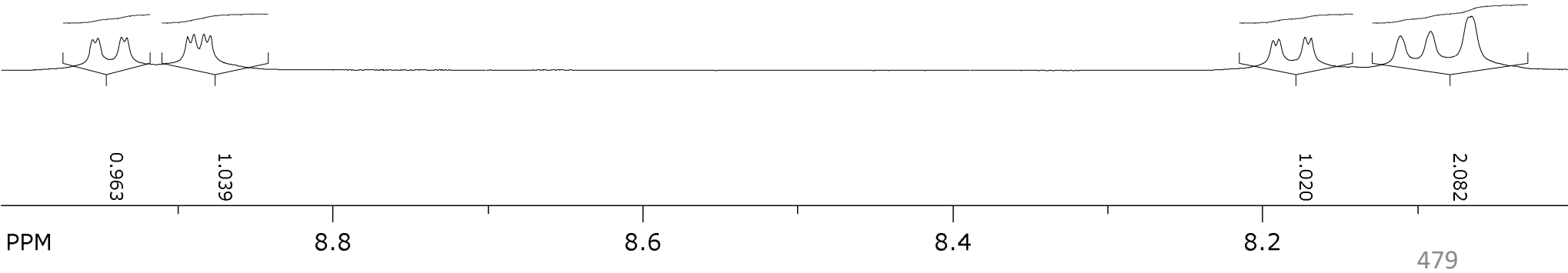
SpinWorks 4: RD-715Re
1H

8.8794
8.8834
8.8898
8.9332
8.9366
8.9518
8.9552

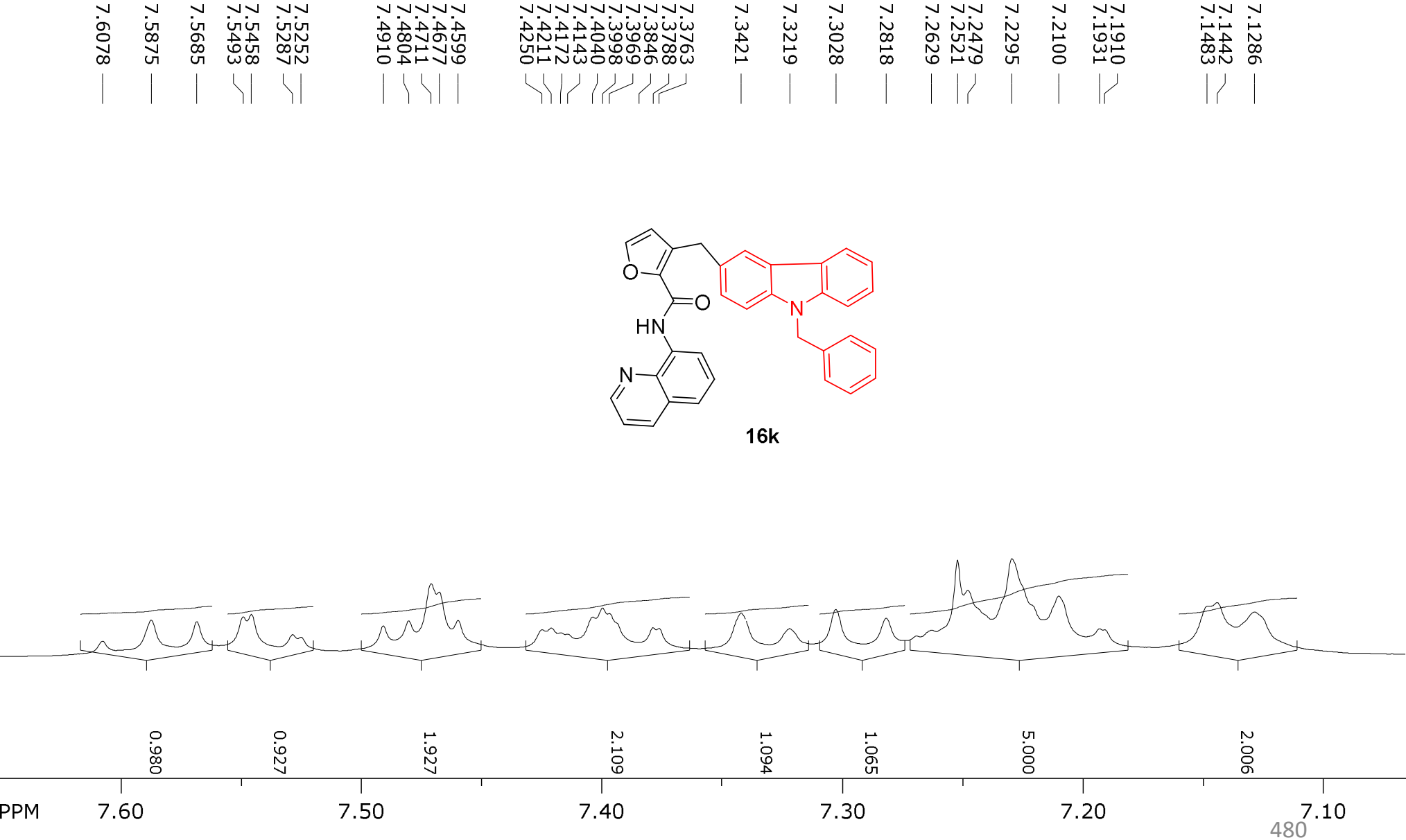
8.0648
8.0666
8.0916
8.1109
8.1686
8.1726
8.1894
8.1933



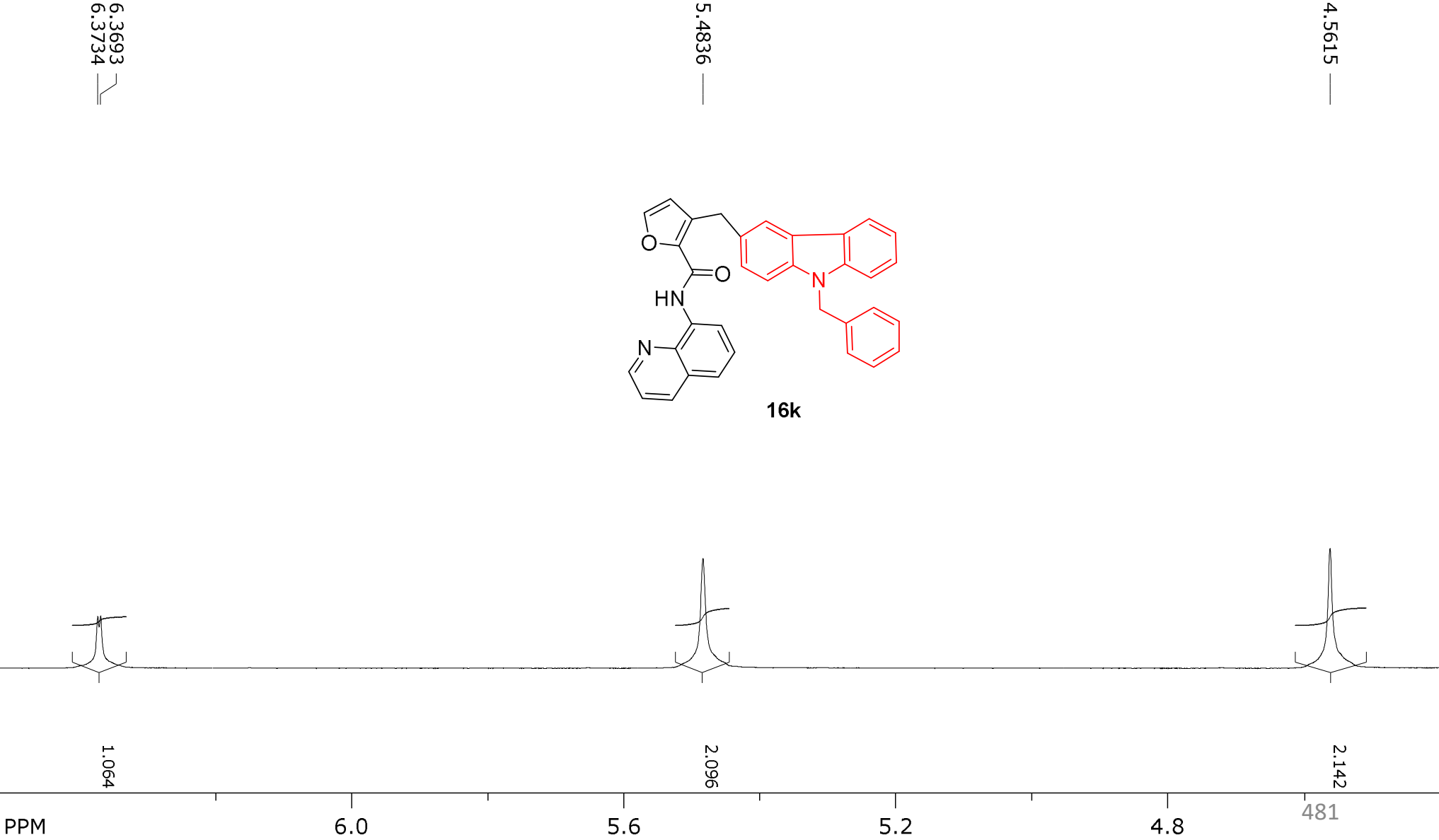
16k



SpinWorks 4: RD-715Re
1H



SpinWorks 4: RD-715Re
1H



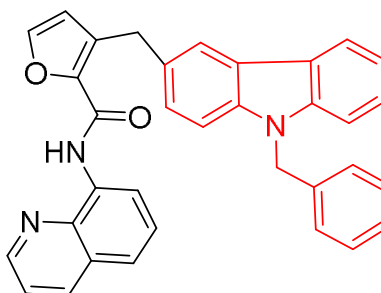
SpinWorks 4: RD-715
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

108.803
108.881
114.743
116.474
119.011
120.420
121.552
121.619
123.196
123.798
128.008
128.008
130.838
133.237
134.462
136.292
137.217
138.713
139.434
140.878
142.025
143.125
148.334
157.772

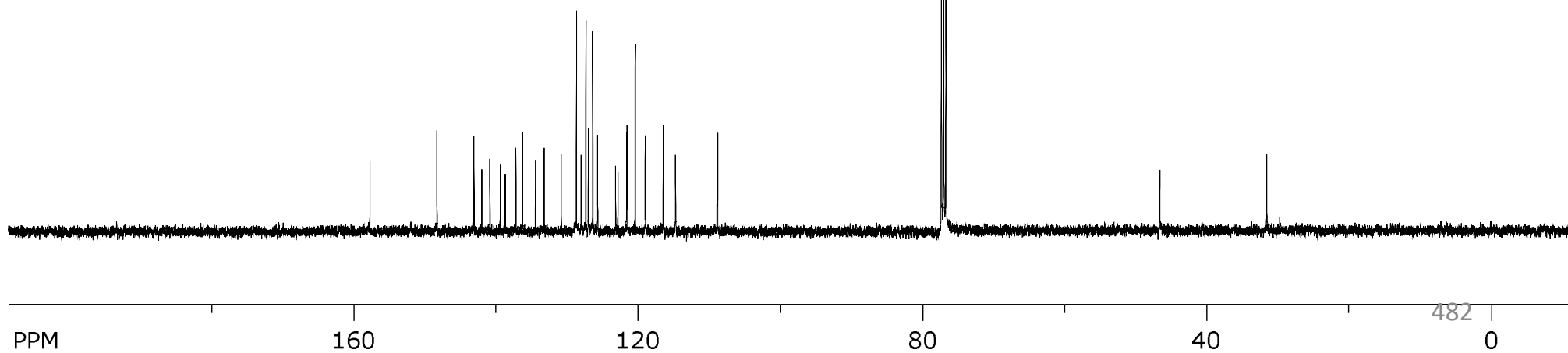
76.683
77.000
77.318

46.567

31.513



16k



SpinWorks 4: RD-715
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 20

157.772 —

148.334 —

143.125 —

142.025 —

140.878 —

139.434 —

138.713 —

137.217 —

136.292 —

134.462 —

133.237 —

130.838 —

128.702 —

128.030 —

127.373 —

127.017 —

126.403 —

125.710 —

123.176 —

122.860 —

121.619 —

121.552 —

120.420 —

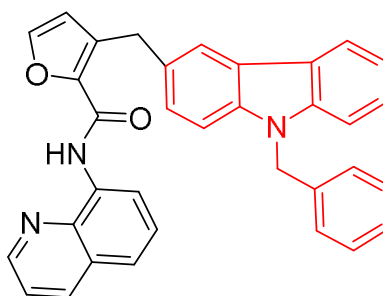
119.011 —

116.474 —

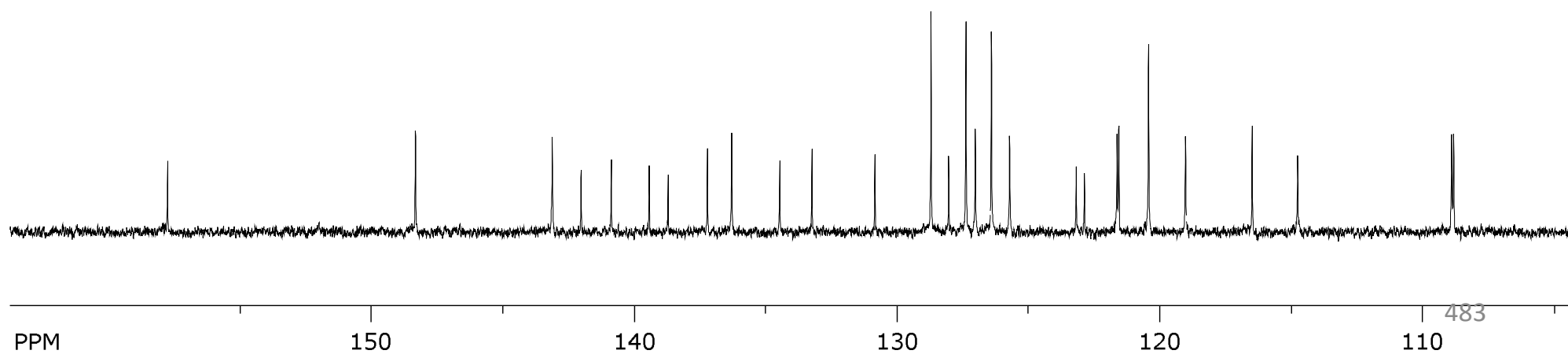
114.743 —

108.881 —

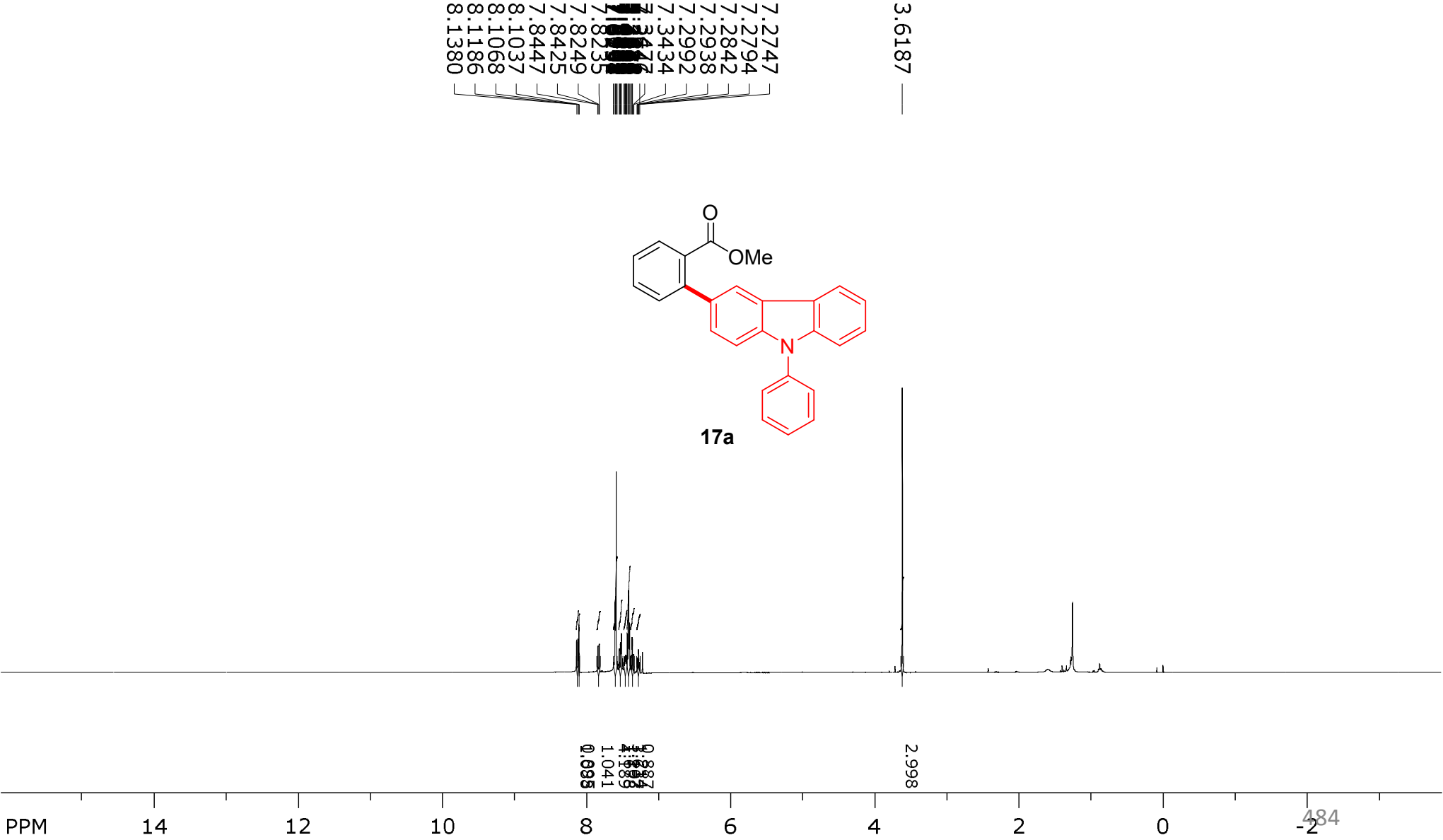
108.803 —



16k



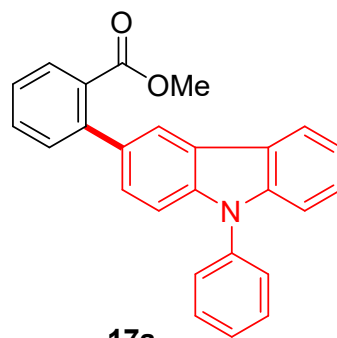
SpinWorks 4: rd-287



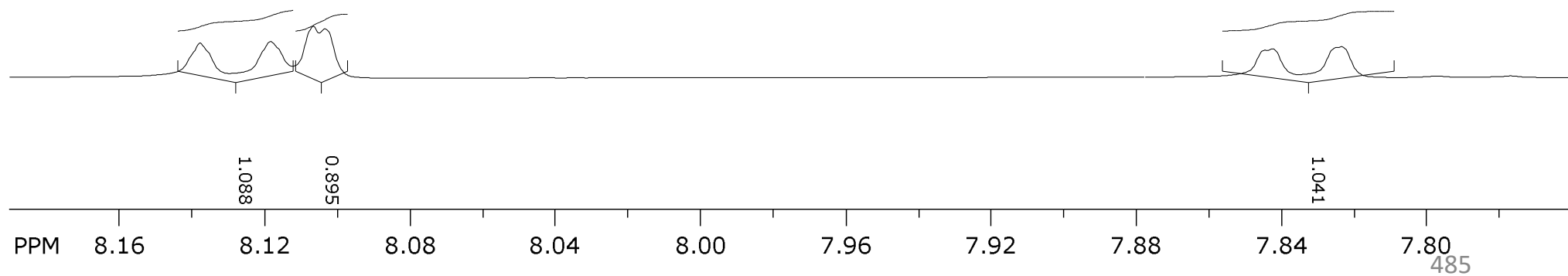
SpinWorks 4: rd-287

8.1037
8.1068
8.1186
8.1380

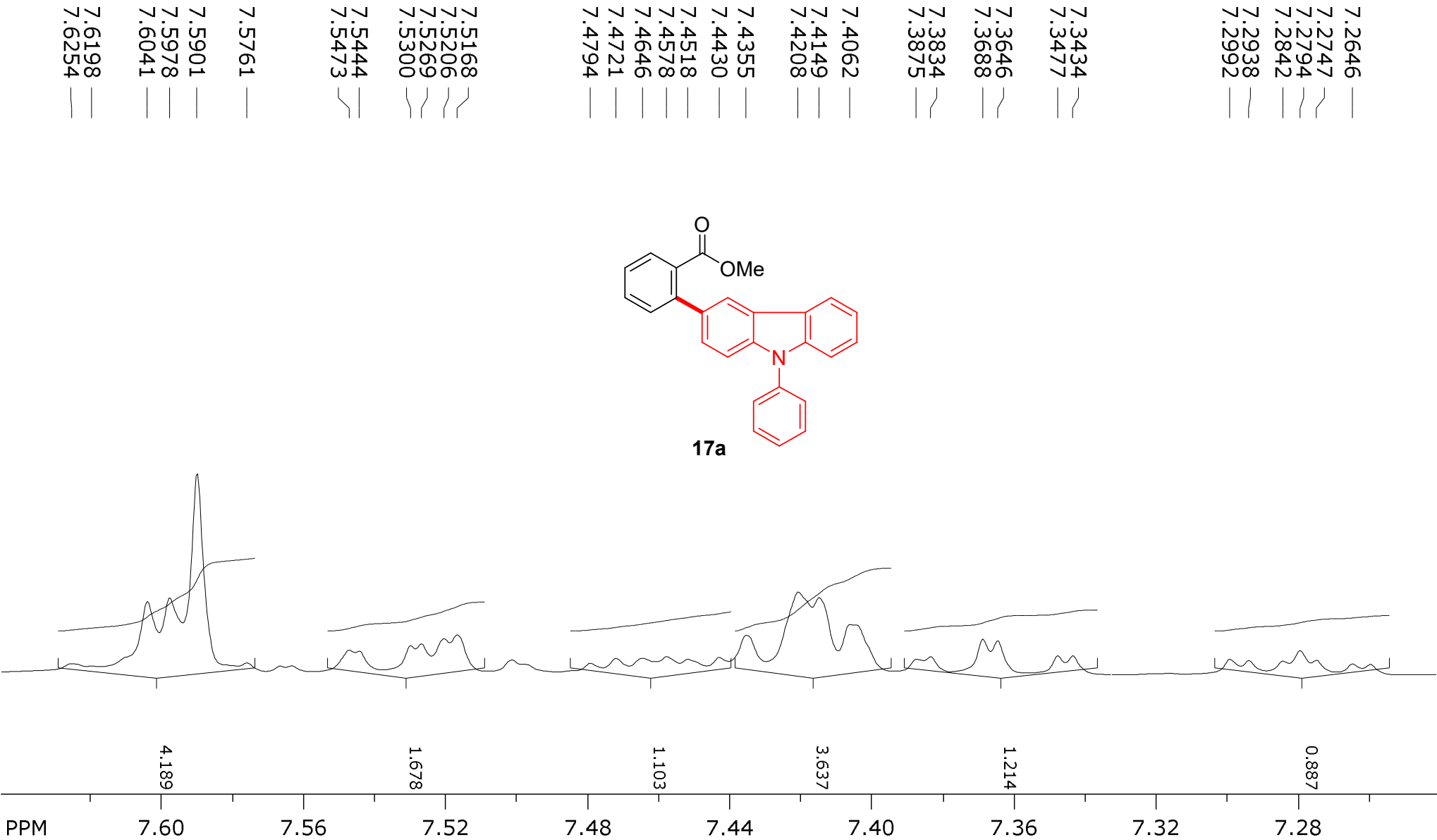
7.8235
7.8249
7.8425
7.8447



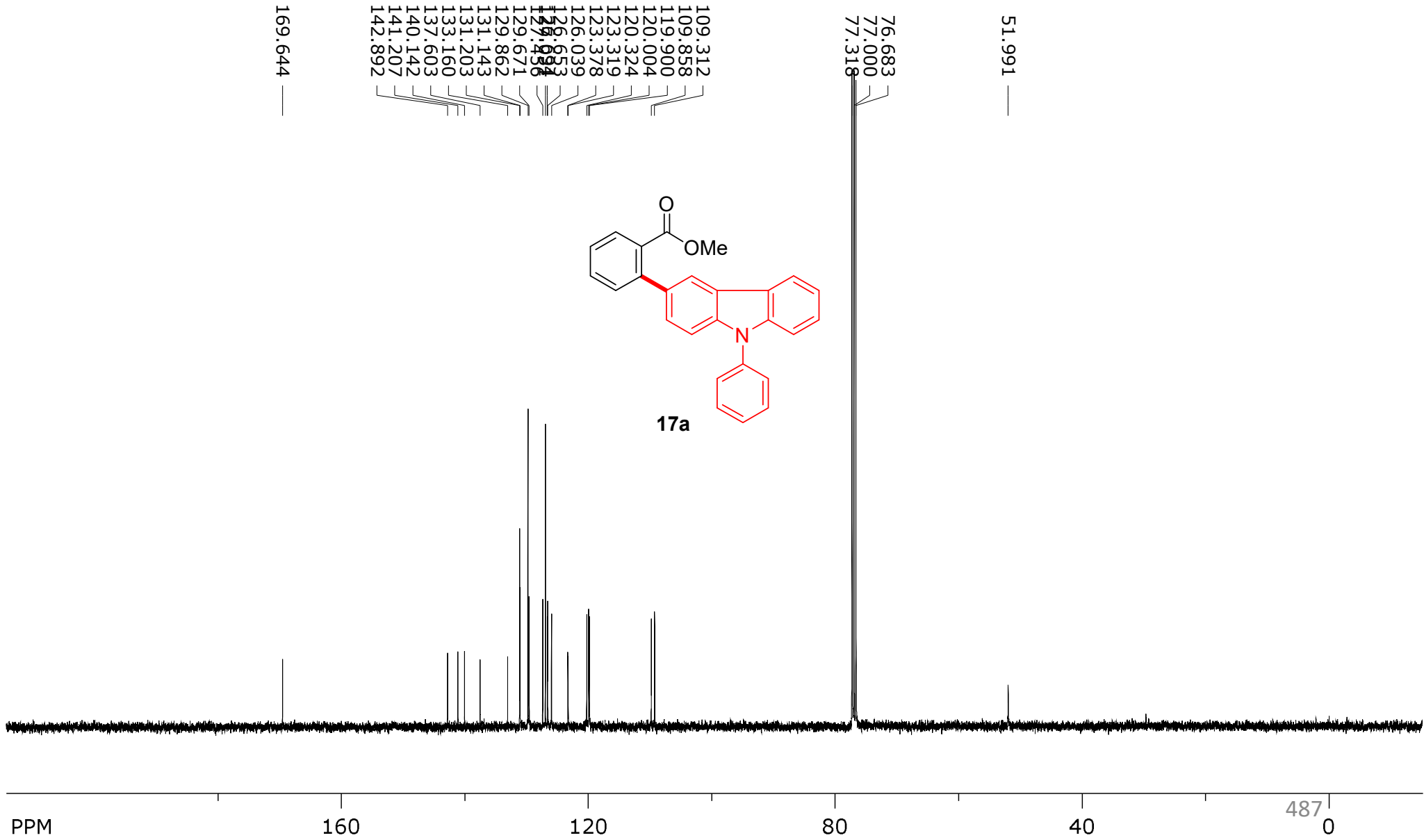
17a



SpinWorks 4: rd-287



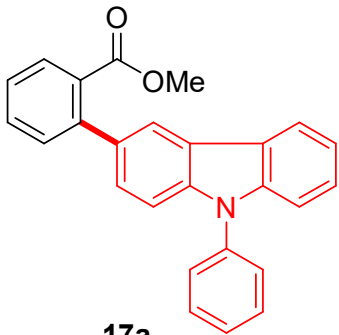
SpinWorks 4: RD 287
13 C



SpinWorks 4: RD 287
13 C

169.644

109.312
109.858
119.900
120.004
120.324
123.319
123.378
126.039
126.653
126.694
127.031
127.456
129.671
129.862
131.143
131.203
133.160
137.603
140.142
141.207
142.892



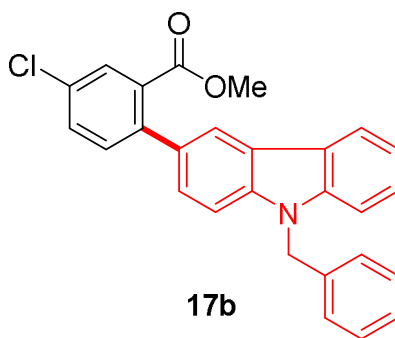
17a

PPM 170 160 150 140 130 120 110 488

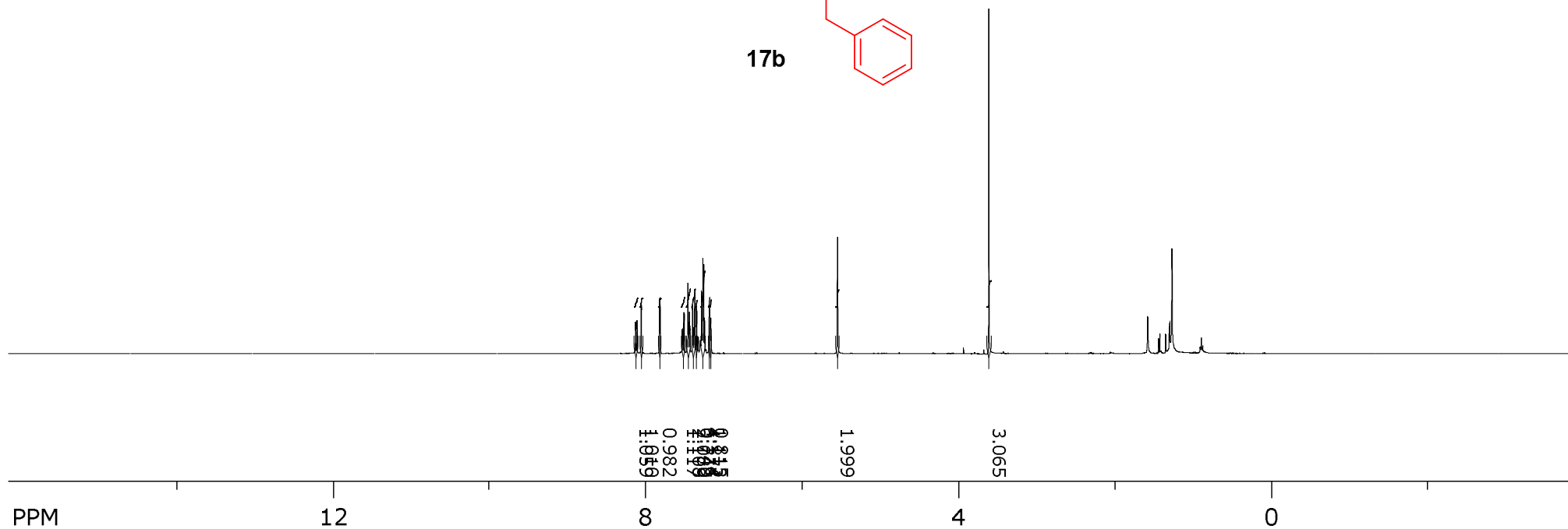
SpinWorks 4: RD 1170
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

5.5466
7.1692
7.1849
7.1893
7.2492
7.2600
7.2689
7.2839
7.3000
7.3000
7.3000
7.3000
7.5299
7.5356
7.8173
7.8228
8.0572
8.0604
8.1126
8.1319

3.6101



17b



SpinWorks 4: RD 1170

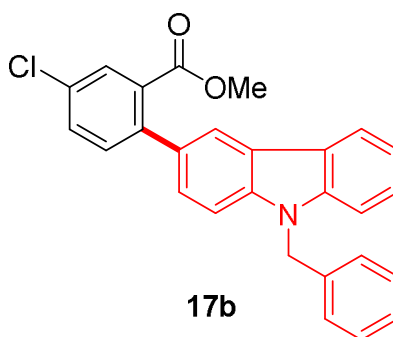
PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 5

8.1319

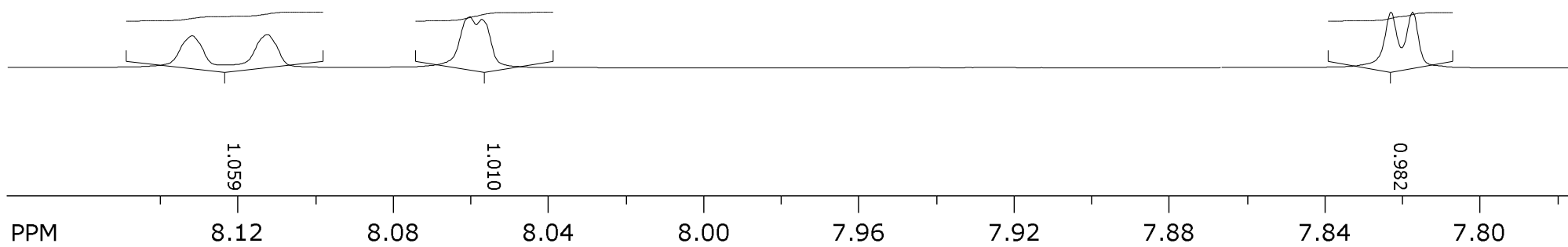
8.1126

8.0572
8.0604

7.8173
7.8228

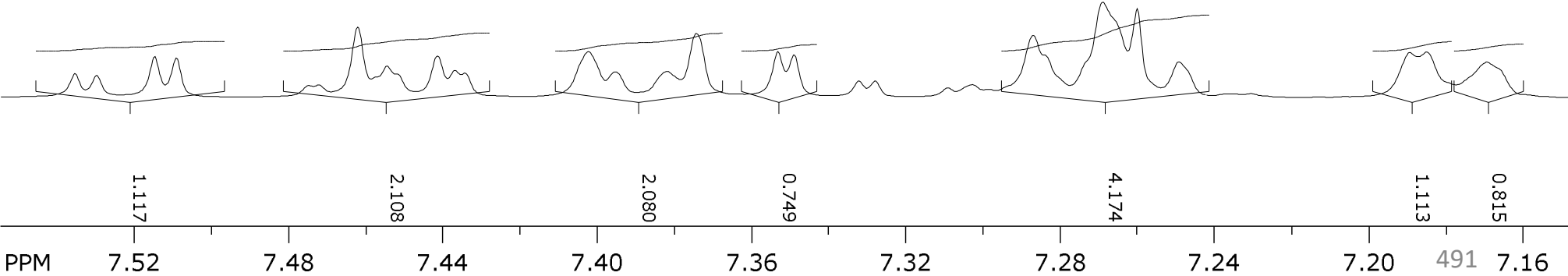
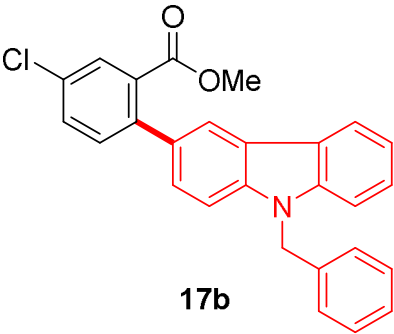


17b



SpinWorks 4: RD 1170
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

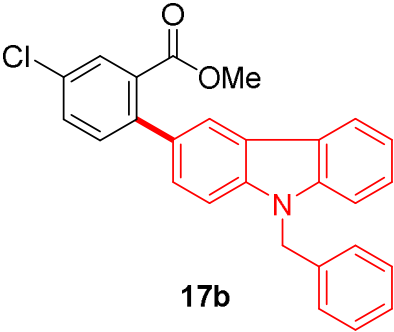
7.5356	7.5299	7.5149	7.5092	7.4749	7.4622	7.4546	7.4520	7.4415	7.4370	7.4344	7.4024	7.3954	7.3820	7.3743	7.3532	7.3490	7.2870	7.2839	7.2689	7.2600	7.2492	7.1893	7.1849	7.1692	
—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—



SpinWorks 4: RD 1170
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

5.5466

3.6101



1.999



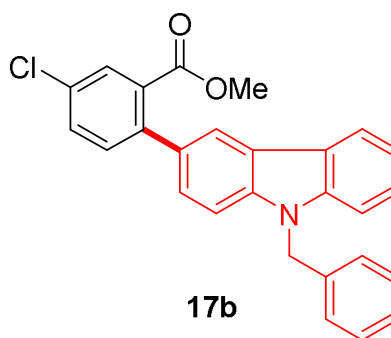
3.065

PPM 5.6 5.2 4.8 4.4 4.0 3.6 492

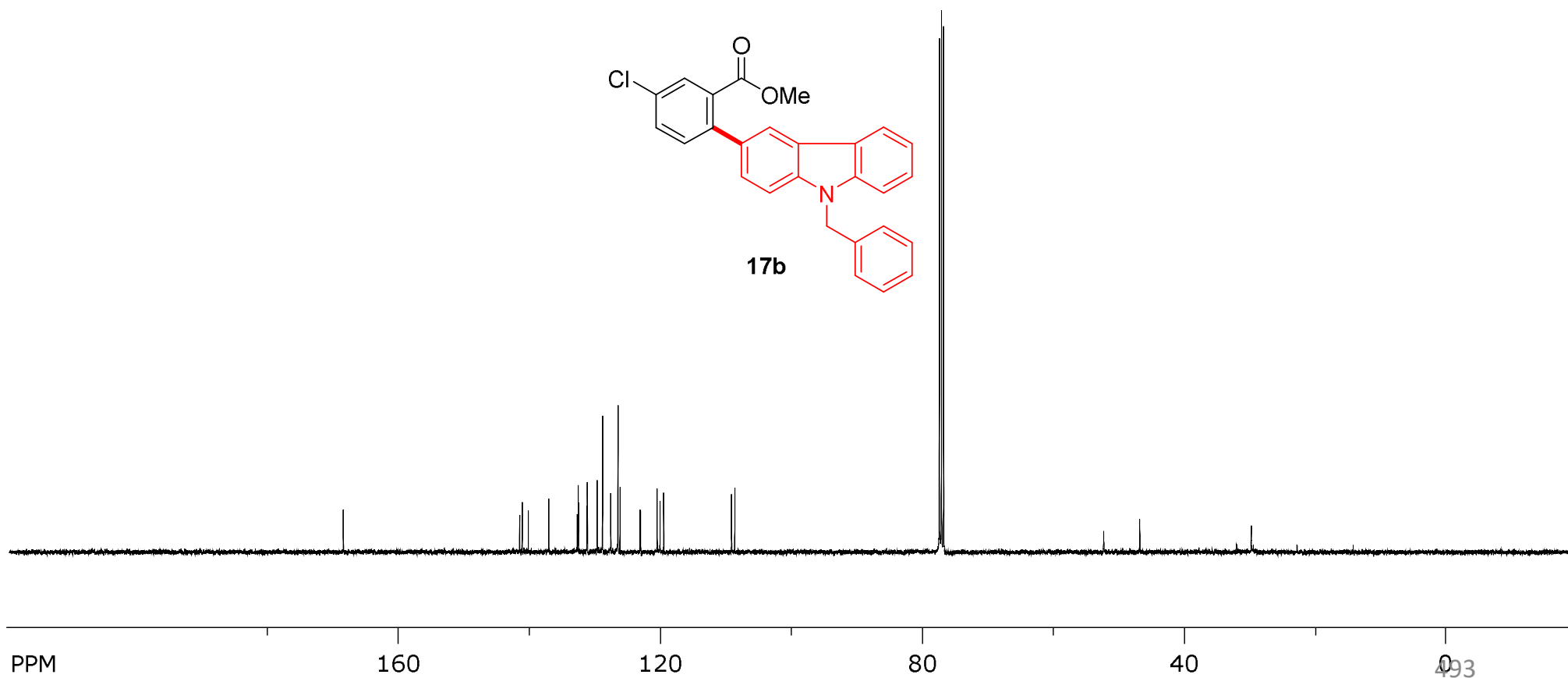
SpinWorks 4: RD 1170

C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

168.396 —
141.466 —
141.076 —
140.126 —
136.993 —
132.651 —
132.513 —
132.480 —
131.173 —
131.114 —
129.804 —
129.542 —
126.437 —
126.135 —
123.072 —
122.970 —
120.448 —
120.014 —
119.456 —
109.091 —
108.600 —
76.702 —
77.020 —
77.337 —
52.246 —
46.720 —

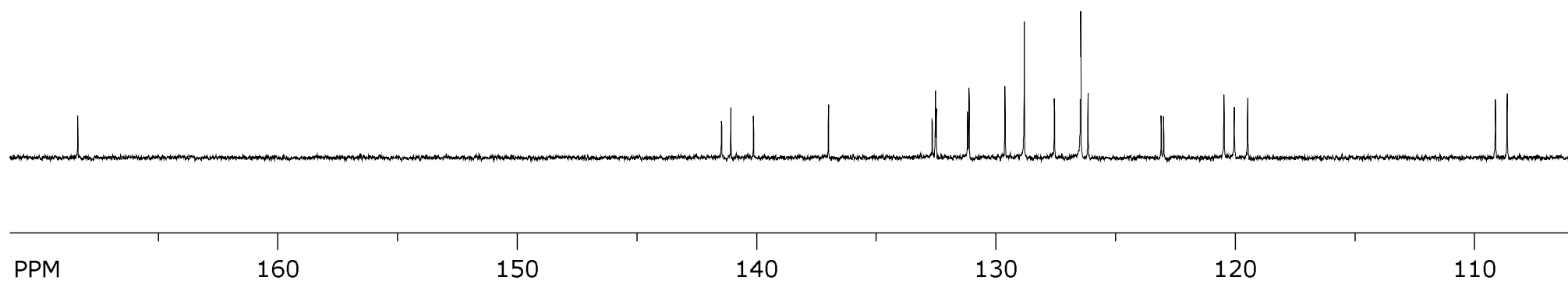
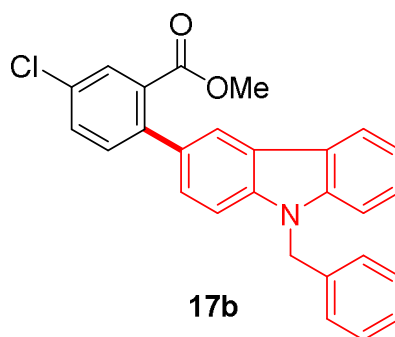


17b



SpinWorks 4: RD 1170
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

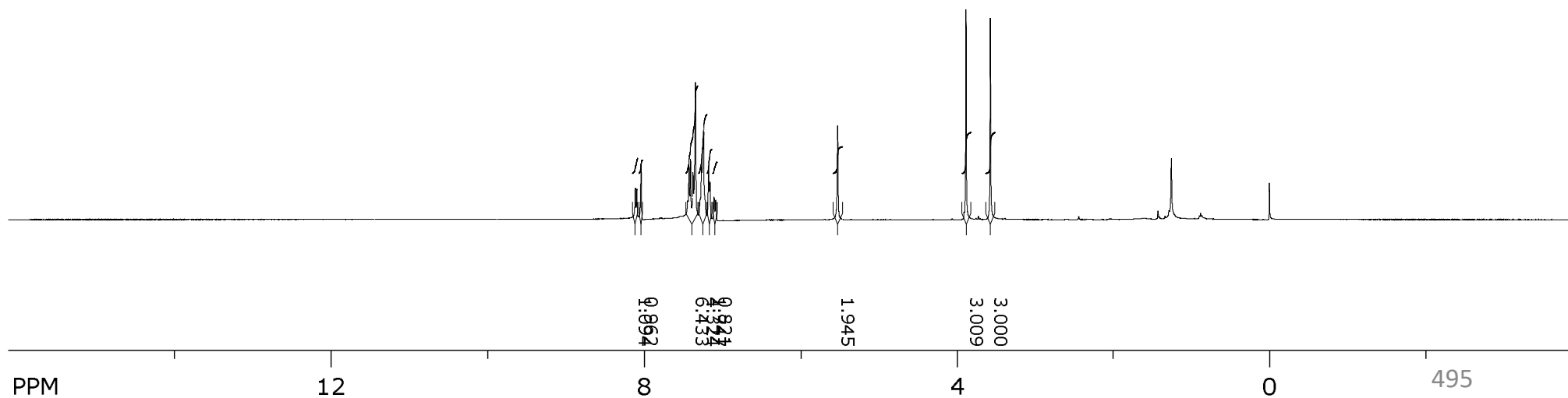
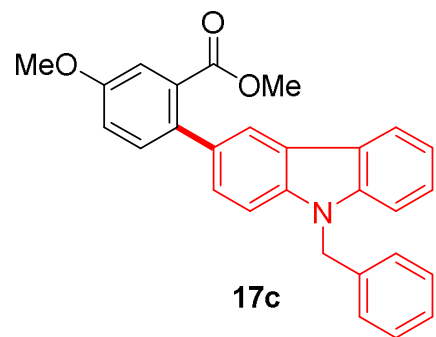
168.396 —
140.126 —
141.076 —
141.466 —
136.993 —
132.651 —
132.513 —
132.480 —
131.173 —
131.114 —
129.606 —
128.804 —
127.542 —
126.437 —
126.135 —
123.072 —
122.970 —
120.448 —
120.014 —
119.456 —
109.091 —
108.600 —



SpinWorks 4: RD 1259

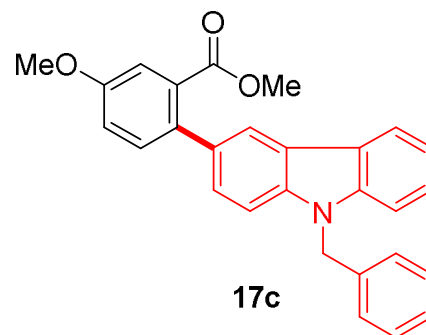
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

3.5714
3.8831
5.5259
7.0875
7.1027
7.1085
7.1597
7.1773
7.2232
7.2898
7.3467
7.3772
7.4082
7.4287
7.4451
8.0423
8.0961
8.1153

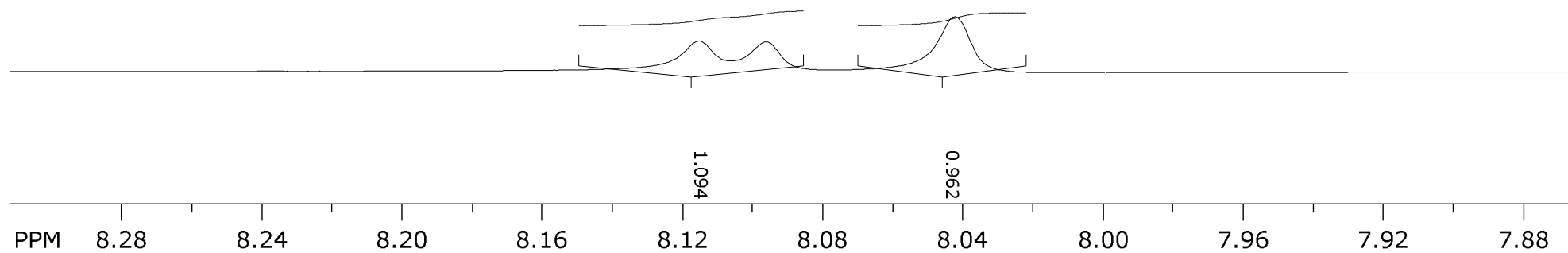


SpinWorks 4: RD 1259
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

8.1153 —
8.0961 —
8.0423 —



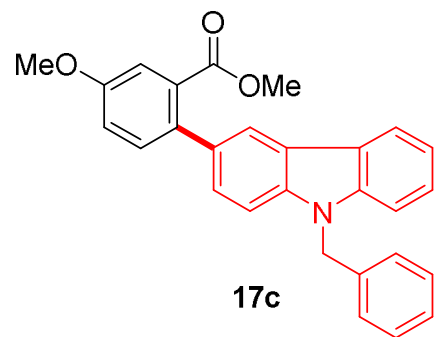
17c



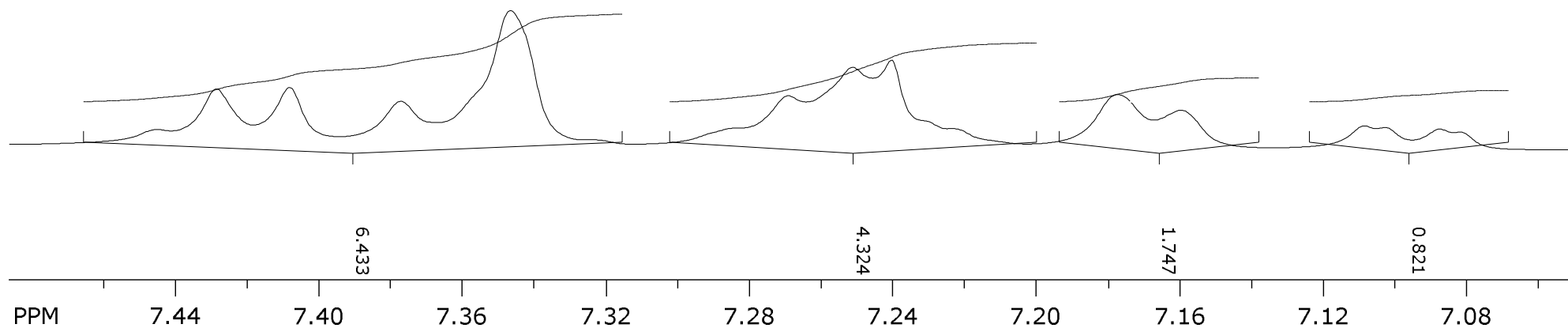
SpinWorks 4: RD 1259

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 31

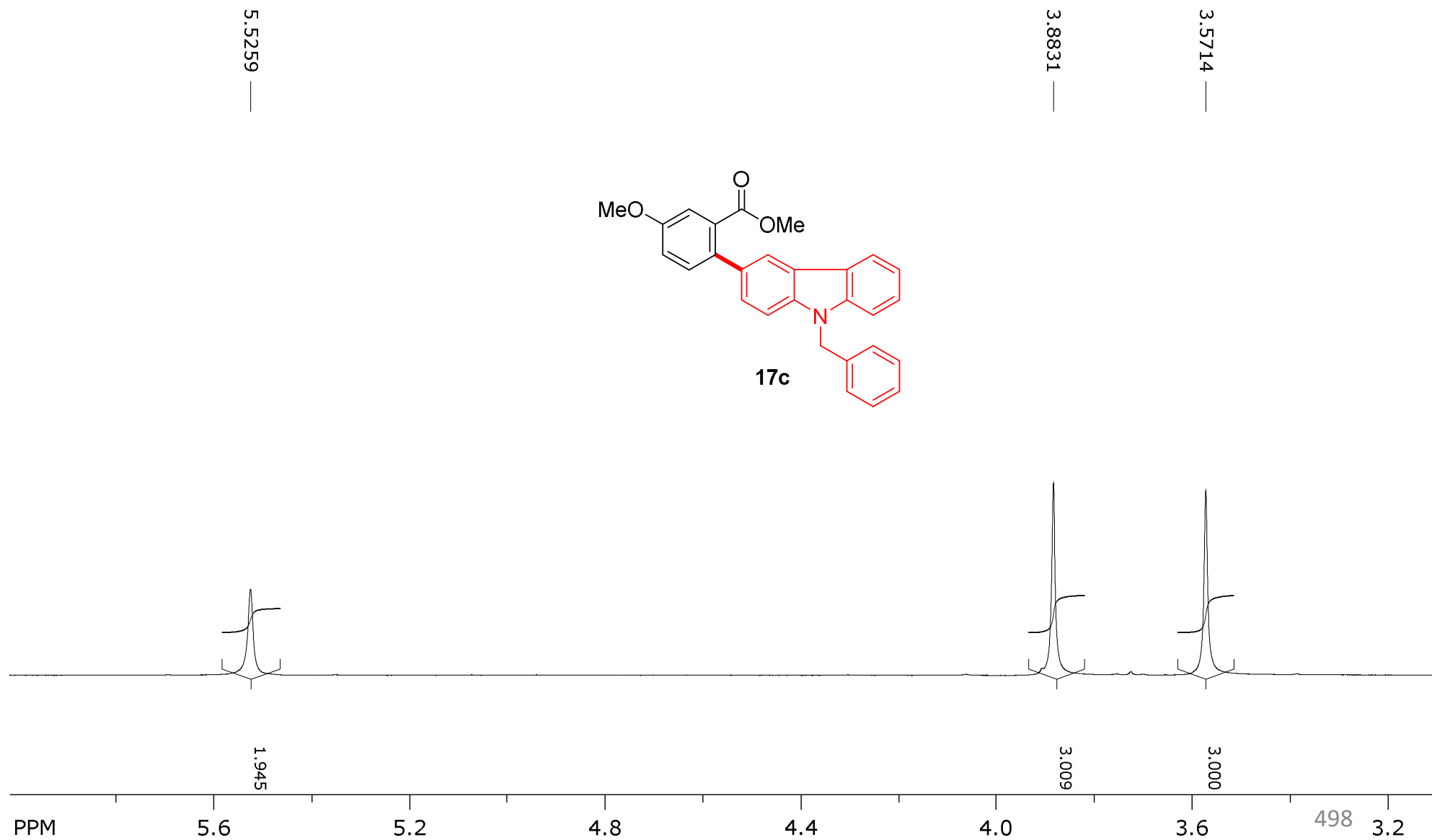
7.4451 —
7.4287 —
7.4082 —
7.3772 —
7.3467 —
7.2835 —
7.2692 —
7.2512 —
7.2404 —
7.2232 —
7.1773 —
7.1597 —
7.1027 —
7.1085 —
7.0875 —
7.0820 —



17c



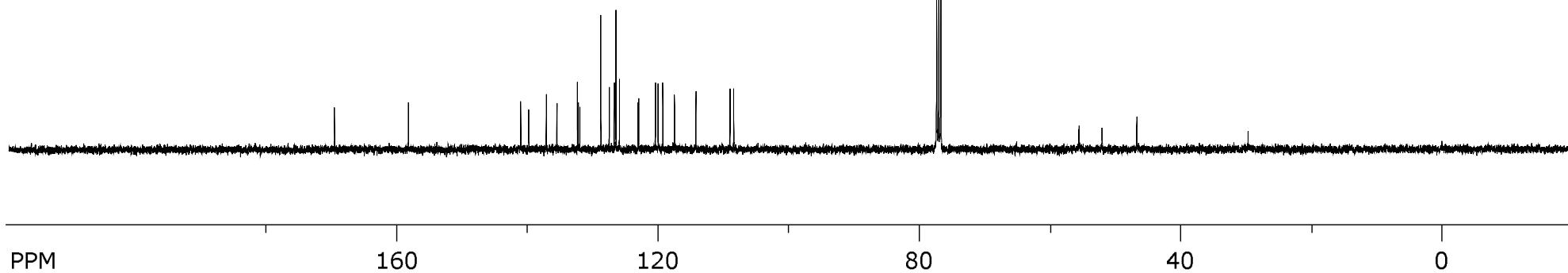
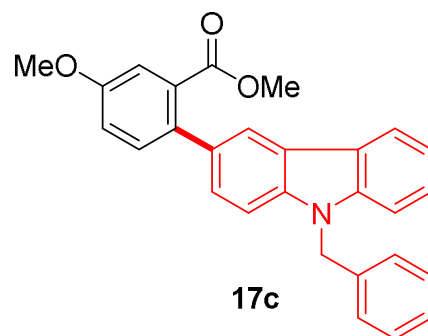
SpinWorks 4: RD 1259
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31



SpinWorks 4: RD 1259

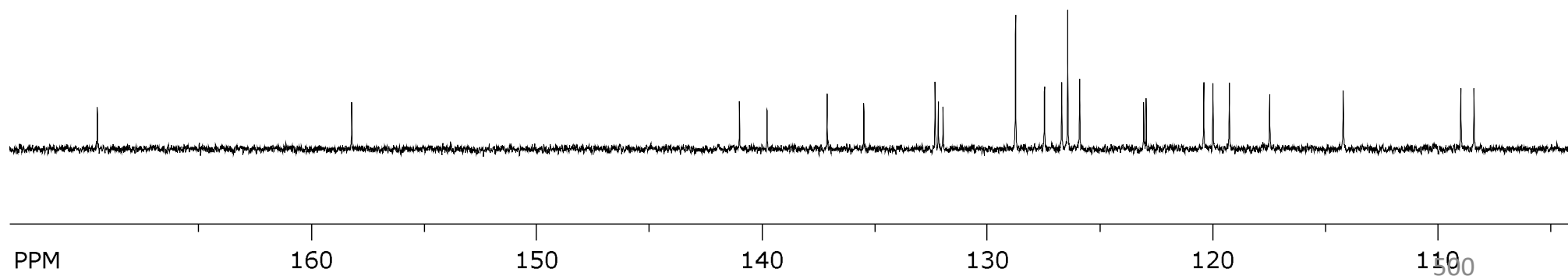
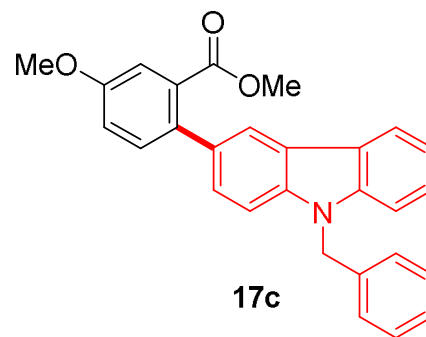
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

169.516 —
158.219 —
141.003 —
139.781 —
137.109 —
135.481 —
132.320 —
132.179 —
131.964 —
128.747 —
127.457 —
126.996 —
126.994 —
123.058 —
122.949 —
120.389 —
119.980 —
119.252 —
117.465 —
114.197 —
108.976 —
108.392 —
77.337 —
77.020 —
76.702 —
55.573 —
52.022 —
46.698 —



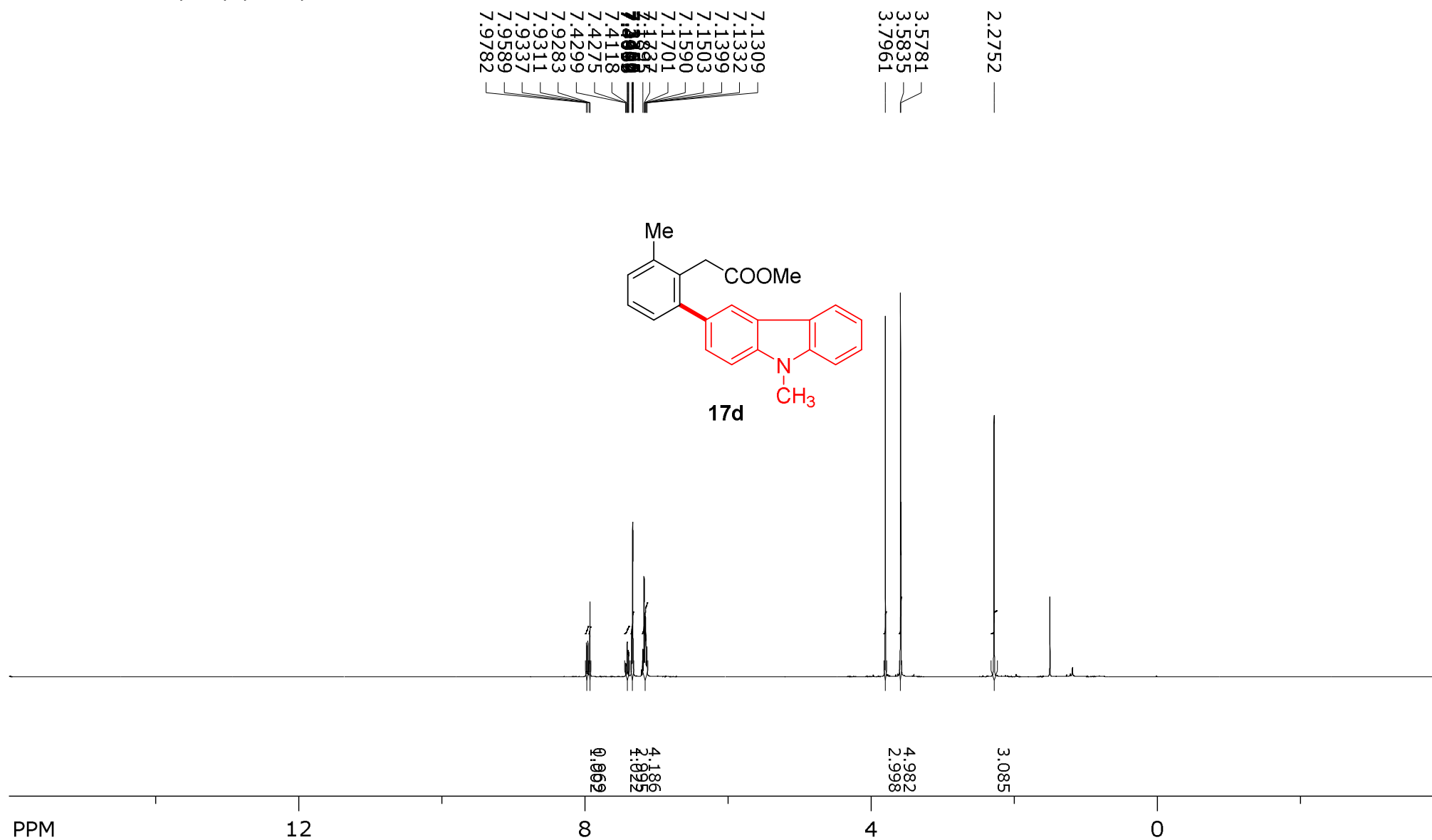
SpinWorks 4: RD 1259
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

169.516 —
158.219 —
141.003 —
139.781 —
137.109 —
135.481 —
132.320 —
132.179 —
131.964 —
128.747 —
127.457 —
126.696 —
126.434 —
125.901 —
123.058 —
122.949 —
120.389 —
119.980 —
119.252 —
117.465 —
114.197 —
108.976 —
108.392 —



SpinWorks 4: RD 1250

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14



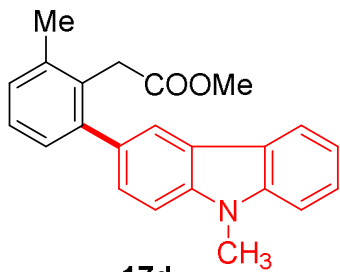
SpinWorks 4: RD 1250
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

7.9283
7.9311
7.9337
7.9589
7.9782

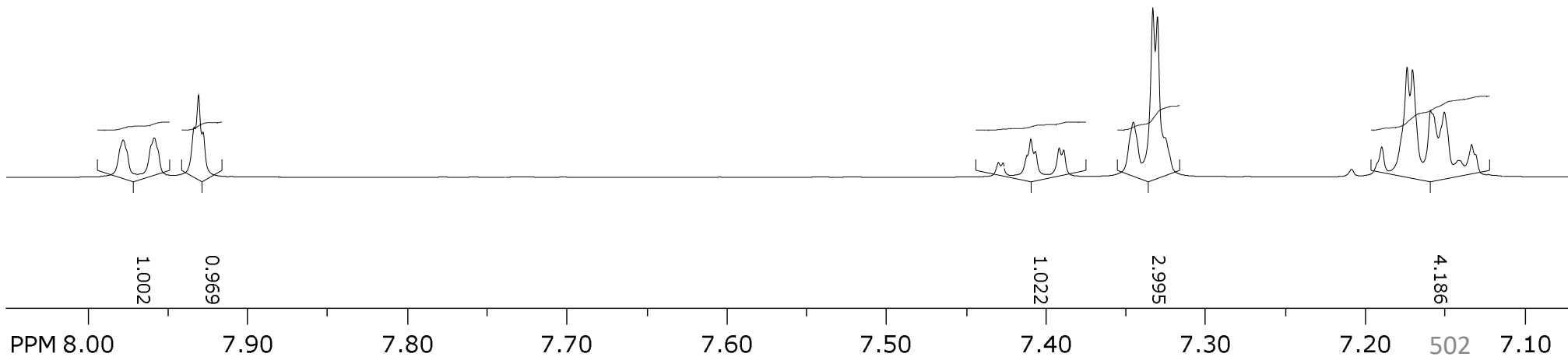
7.3889
7.3917
7.4066
7.4093
7.4118
7.4275
7.4299

7.3255
7.3302
7.3330
7.3453

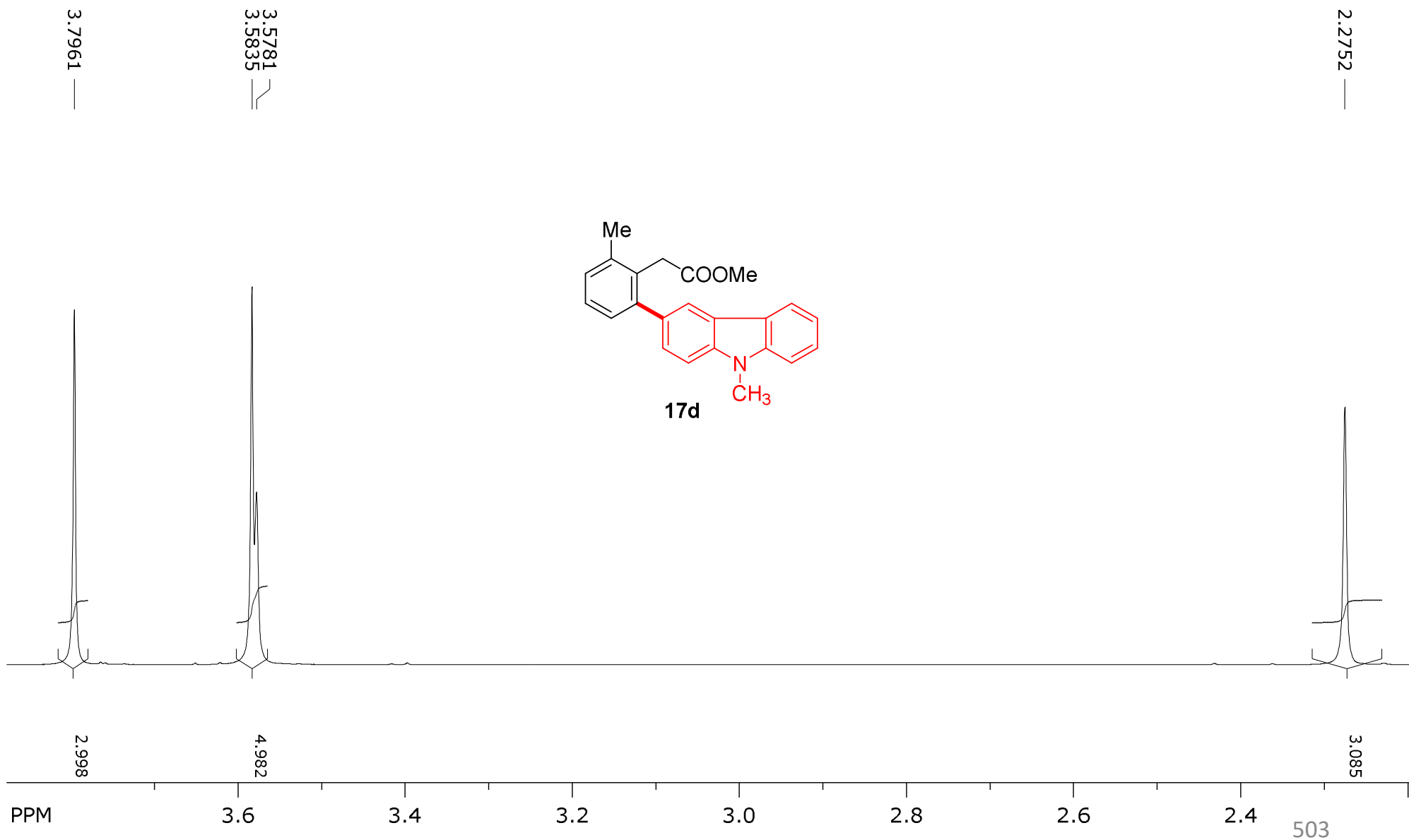
7.1309
7.1332
7.1399
7.1503
7.1590
7.1701
7.1737
7.1895



17d



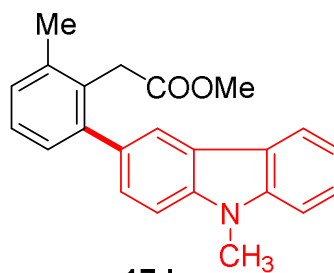
SpinWorks 4: RD 1250
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14



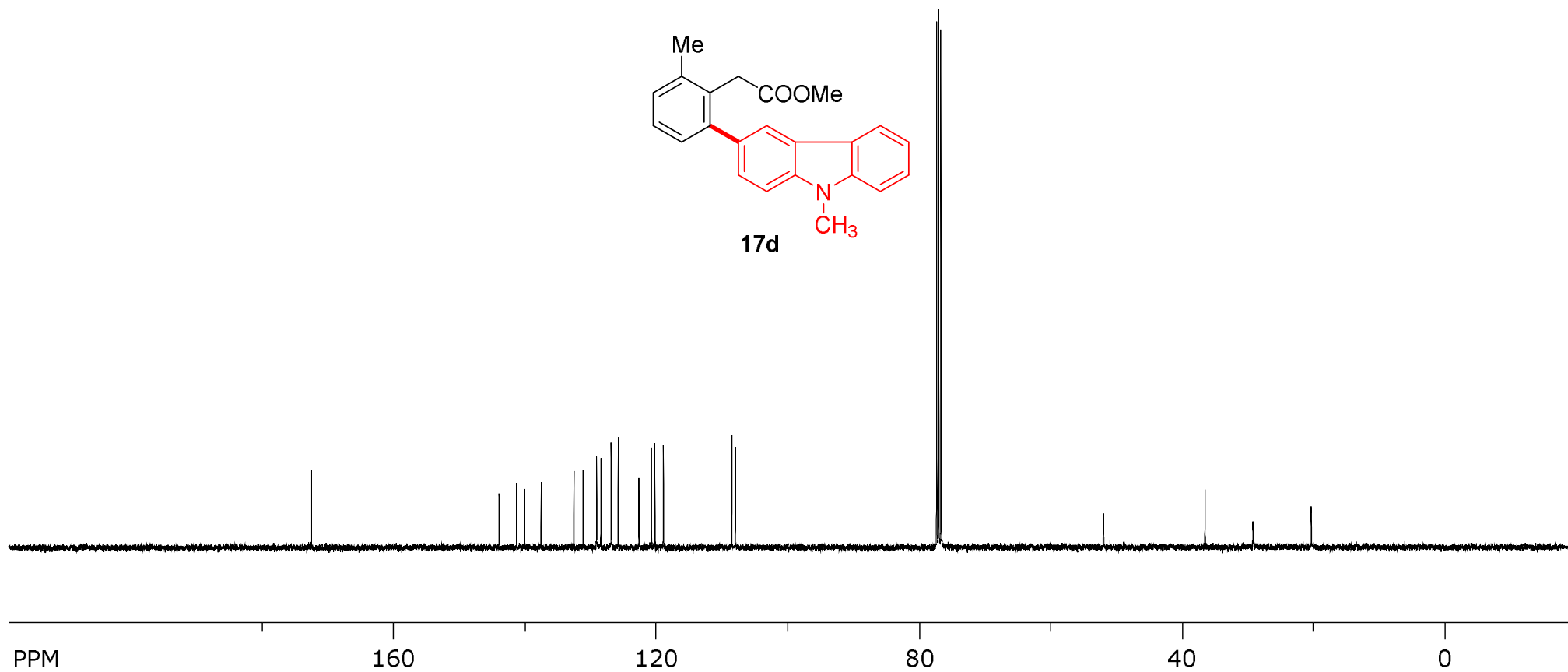
SpinWorks 4: RD 1250

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

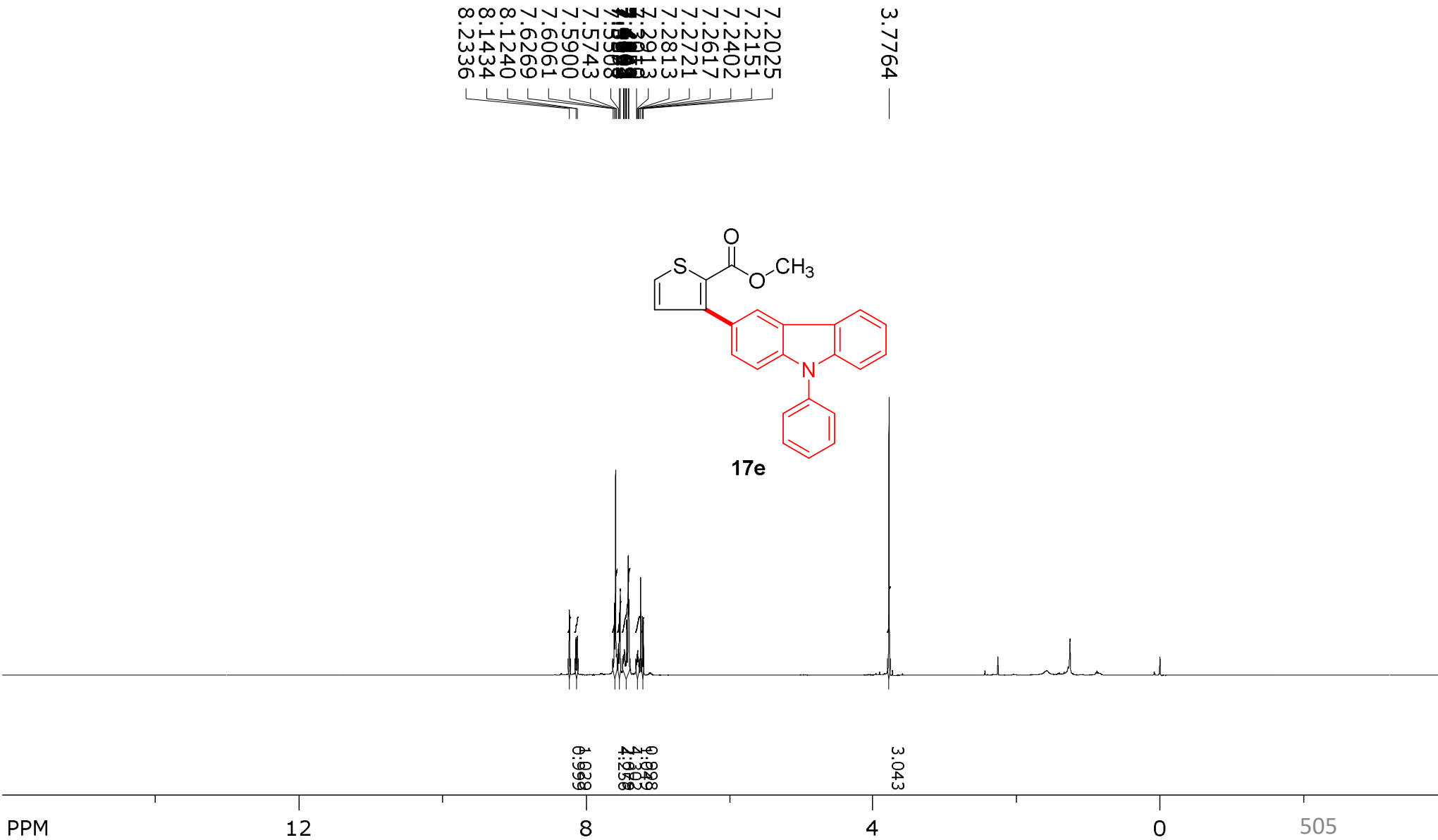
172.533 —
143.979 —
141.342 —
140.080 —
137.597 —
132.600 —
131.200 —
129.117 —
128.475 —
126.912 —
126.816 —
125.848 —
122.684 —
122.562 —
120.794 —
120.248 —
118.951 —
108.540 —
108.002 —
76.703 —
77.020 —
77.338 —
51.922 —
36.463 —
29.161 —
20.291 —



17d



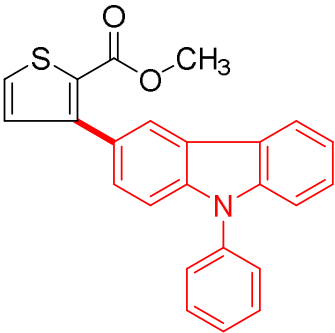
SpinWorks 4: rd-371



8.2336

8.1434

8.1240



17e



PPM

8.24

8.22

8.20

8.18

8.16

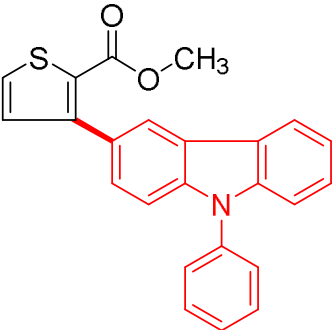
8.14

8.12

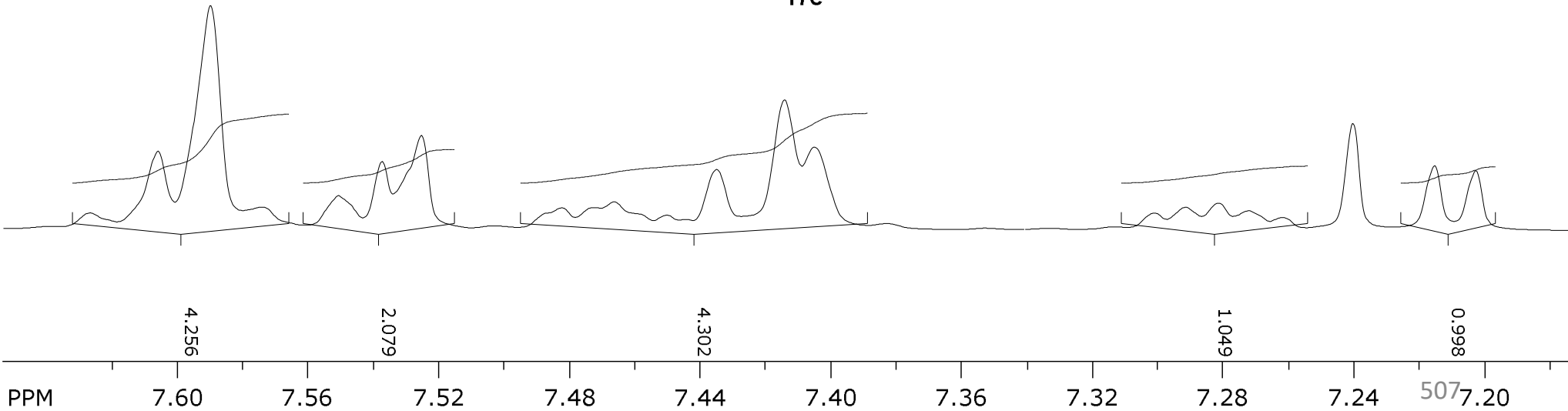
8.10

SpinWorks 4: rd-371

7.2025 —
7.2151 —
7.2402 —
7.2617 —
7.2721 —
7.2813 —
7.2913 —
7.3010 —
7.4052 —
7.4141 —
7.4349 —
7.4445 —
7.4502 —
7.4663 —
7.4727 —
7.4824 —
7.5253 —
7.5374 —
7.5508 —
7.5743 —
7.5900 —
7.6061 —
7.6269 —

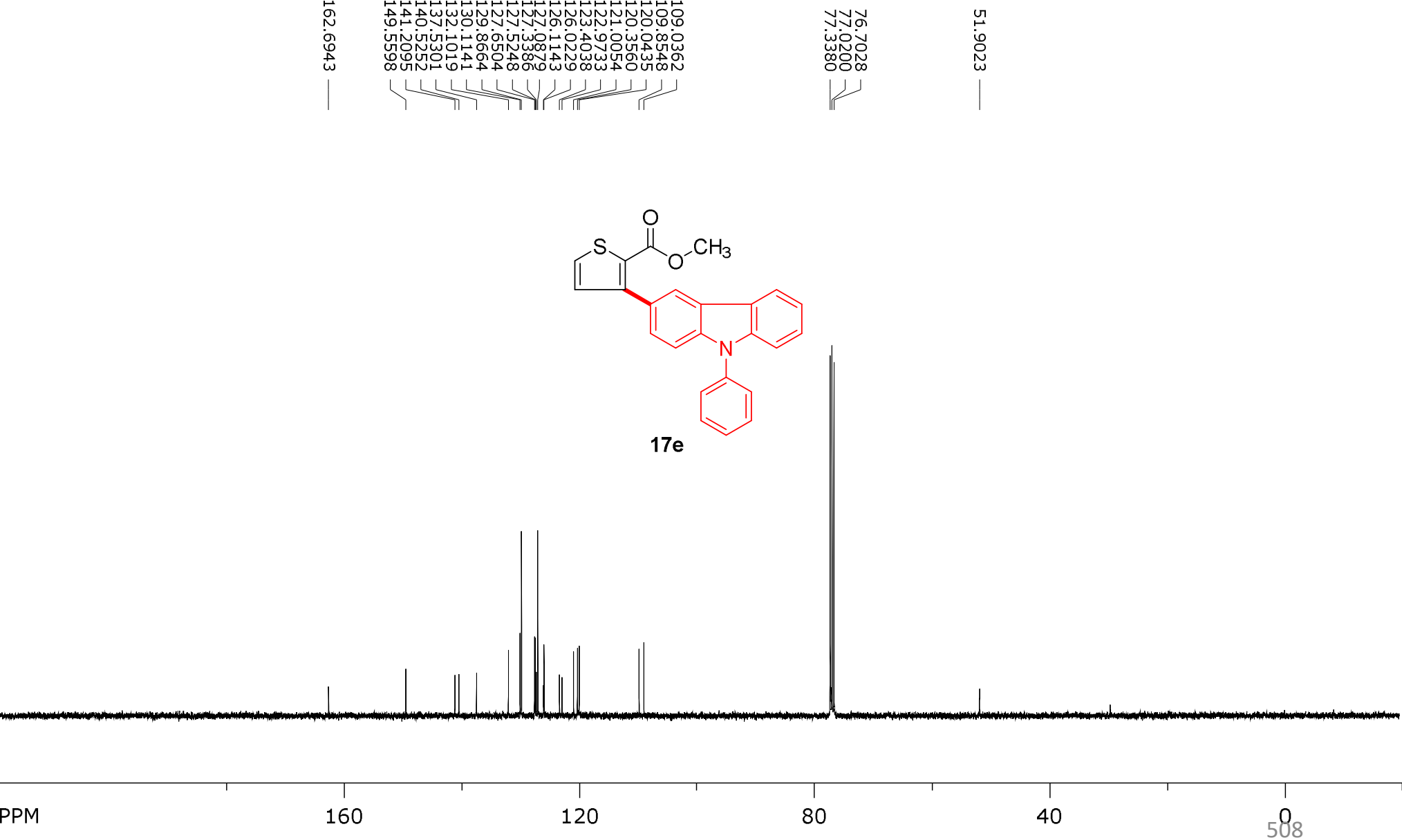


17e



SpinWorks 4: rd-371

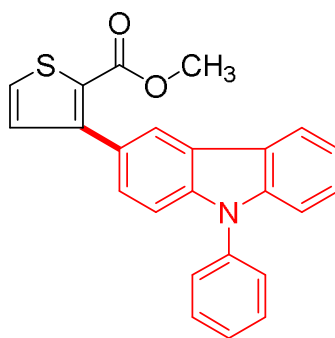
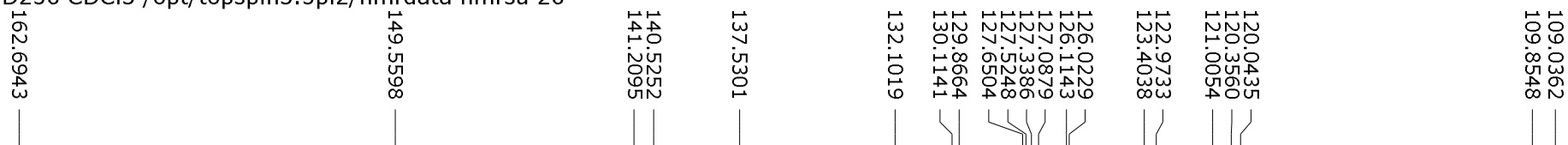
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



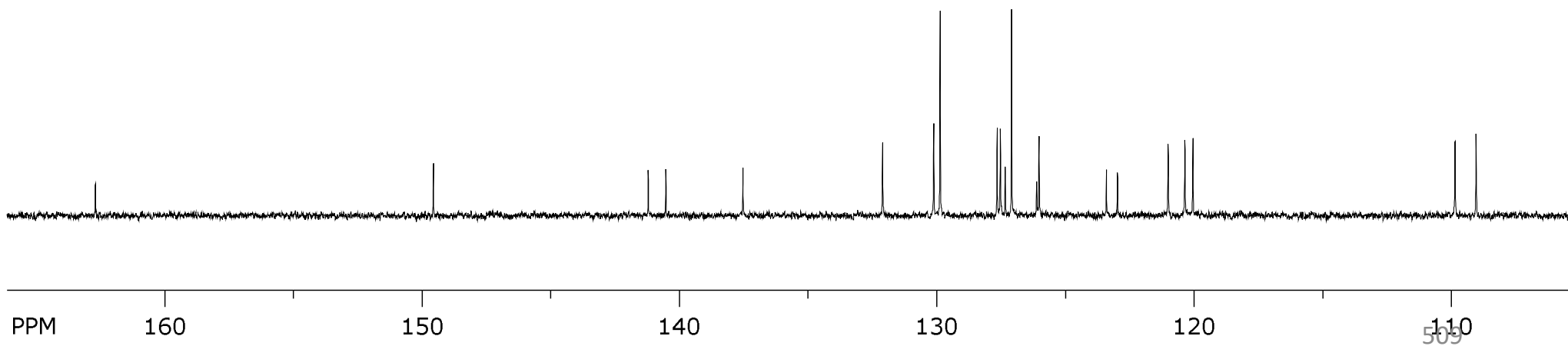
RD-358

SpinWorks 4: rd-371

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 26



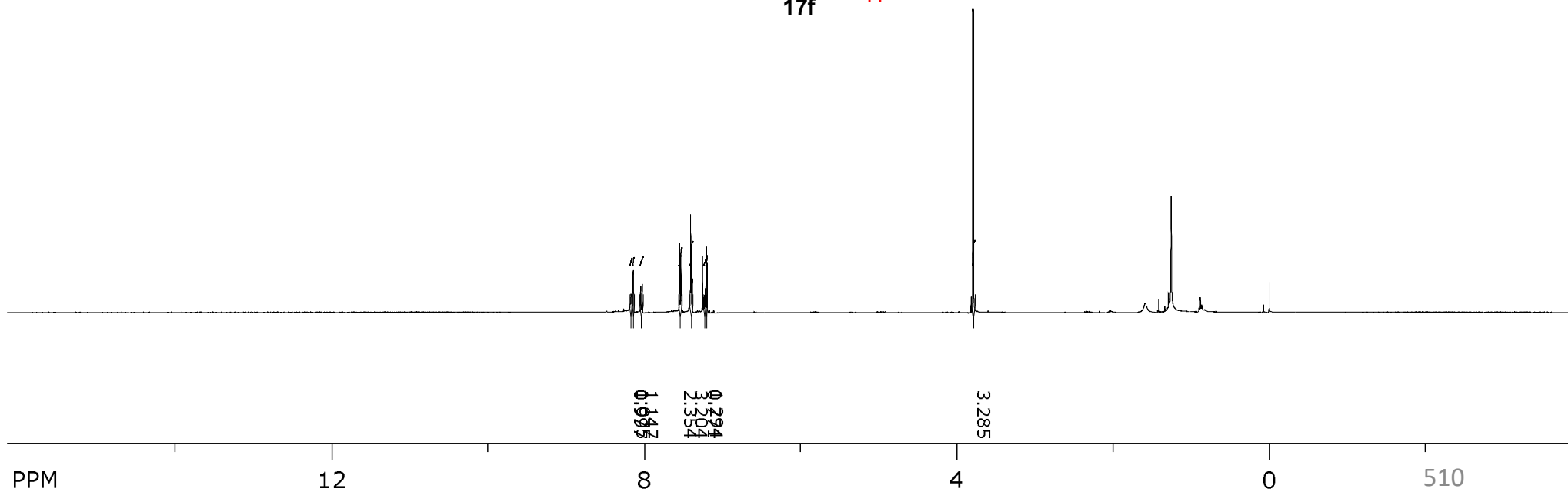
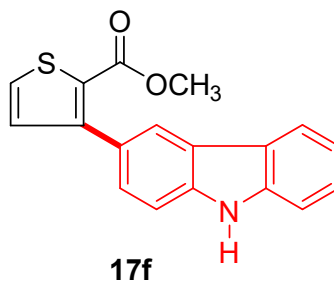
17e



RD-358

SpinWorks 4: rd-258

3.7853
7.1929
7.1965
7.2057
7.2169
7.2260
7.2273
7.3368
7.3388
7.3408
7.5433
7.5465
8.0258
8.0453
8.1371
8.1390
8.1410
8.1690



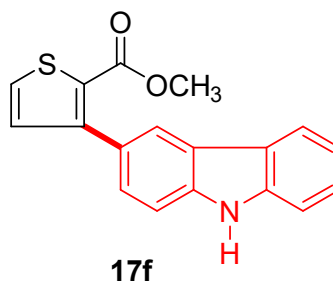
RD-358
SpinWorks 4: rd-258

8.1690

8.1371
8.1390
8.1410

8.0453

8.0258



17f

0.997

1.075

1.147

PPM

8.16

8.12

8.08

8.04

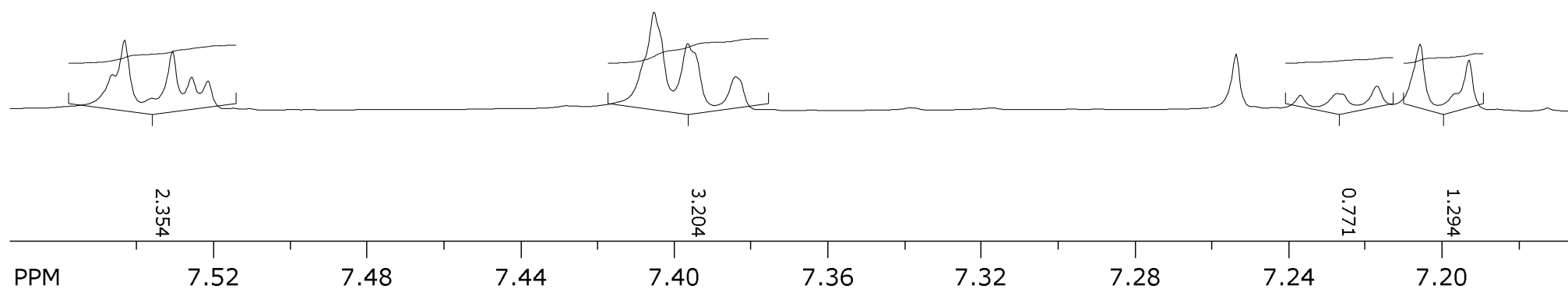
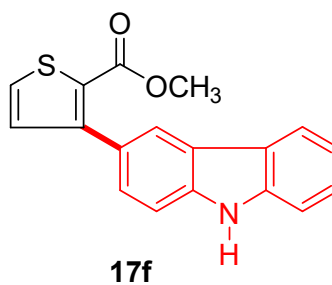
8.00

RD-358
SpinWorks 4: rd-258

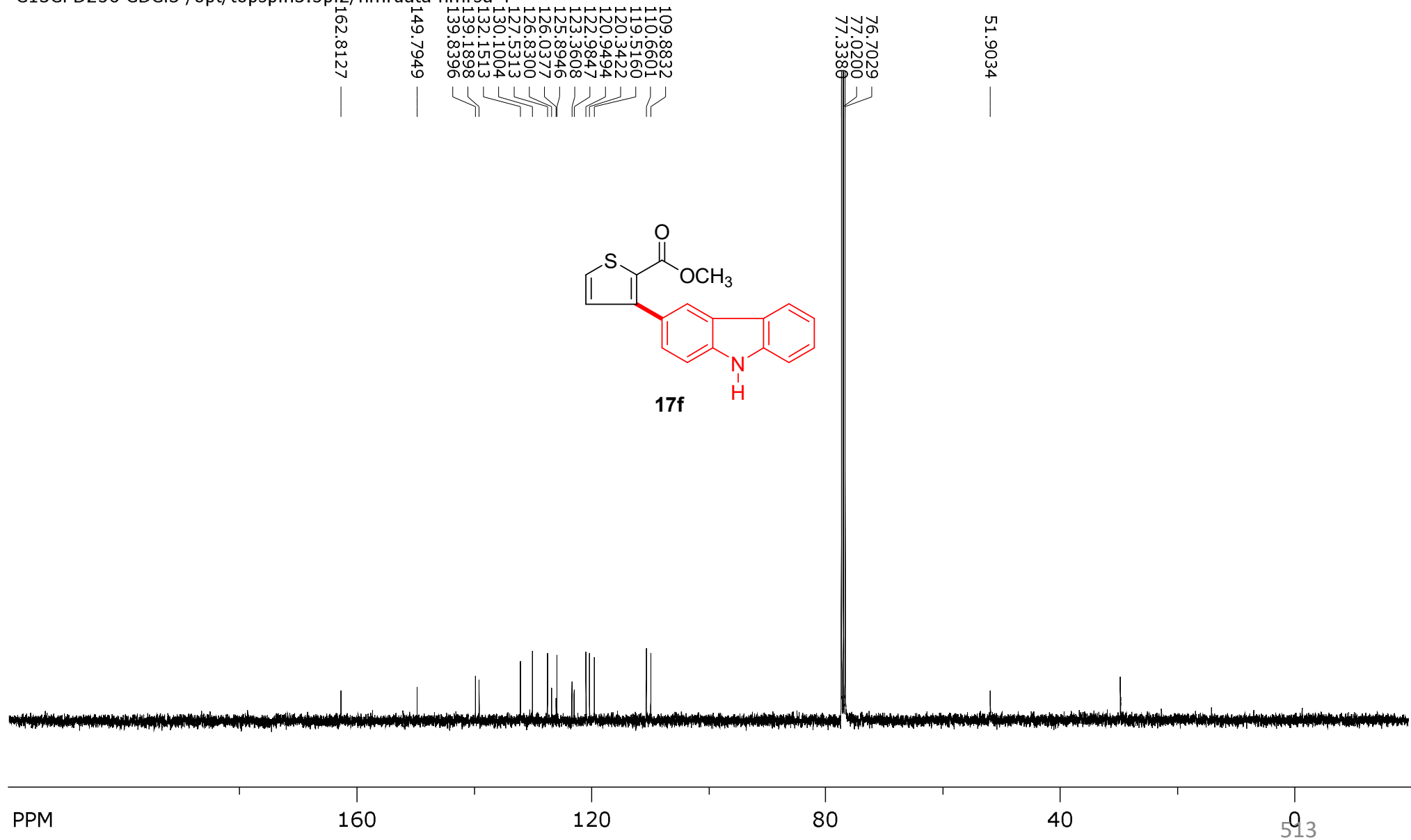
7.5216
7.5258
7.5308
7.5361
7.5433
7.5465

7.3841
7.3965
7.4053

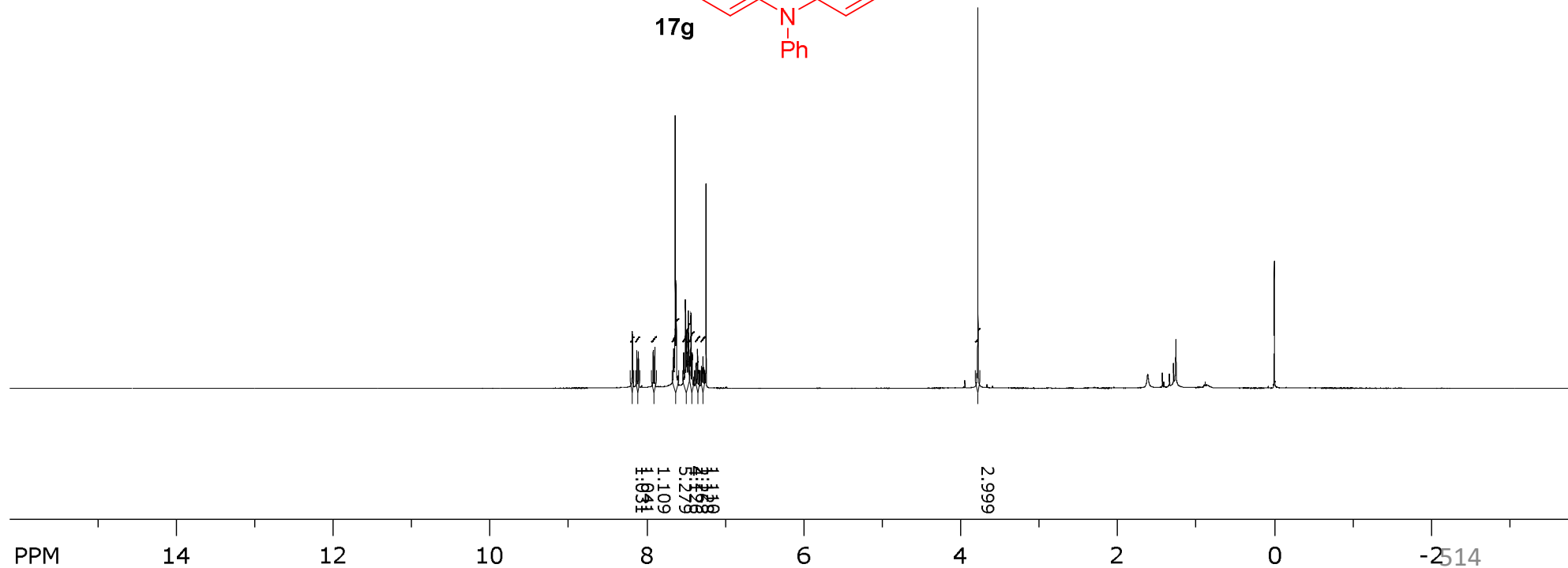
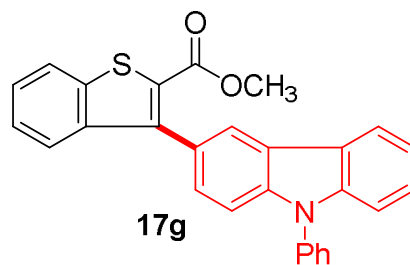
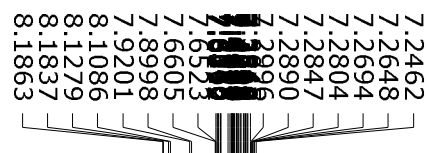
7.1929
7.1965
7.2057
7.2169
7.2260
7.2273
7.2368
7.2536



SpinWorks 4: RD 358
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31



SpinWorks 4: RD 1266

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 31

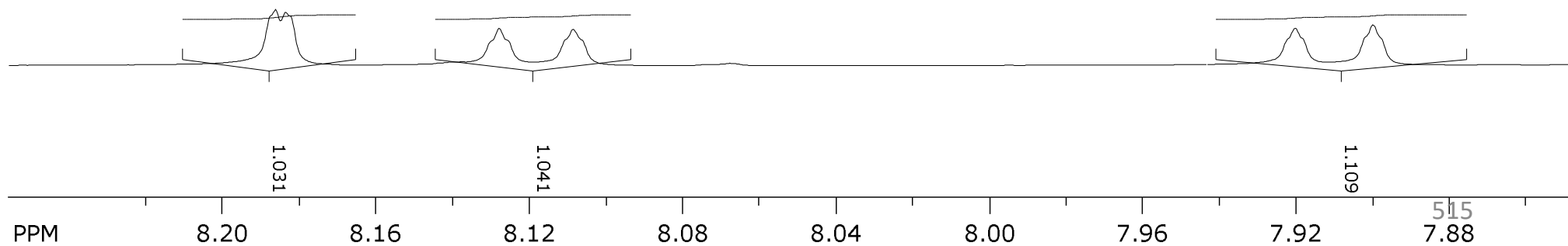
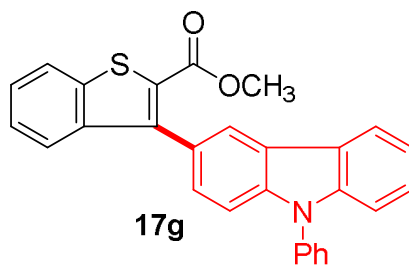
8.1837
8.1863

8.1279

8.1086

7.9201

7.8998



SpinWorks 4: RD 1266
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

7.6043 —
7.6063 —
7.6110 —
7.6260 —
7.6310 —
7.6392 —
7.6499 —
7.6523 —
7.6605 —

7.5307 —

7.5090 —
7.5001 —
7.4944 —
7.4919 —
7.4890 —
7.4861 —
7.4779 —
7.4739 —
7.4711 —
7.4668 —

7.4498 —
7.4456 —
7.4402 —
7.4374 —
7.4244 —
7.4217 —

7.4036 —
7.4009 —

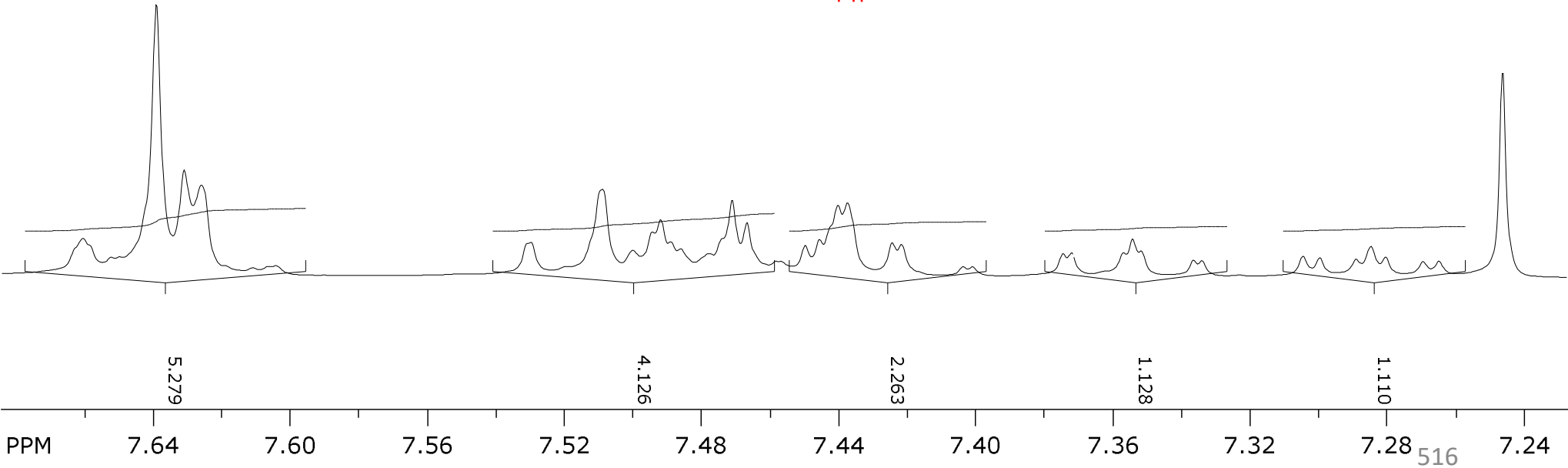
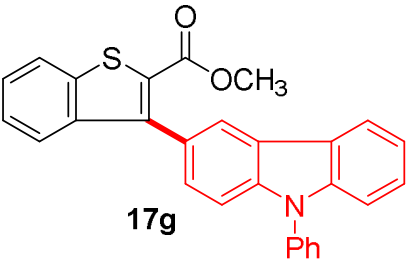
7.3720 —
7.3745 —

7.3569 —
7.3542 —
7.3517 —
7.3364 —
7.3340 —

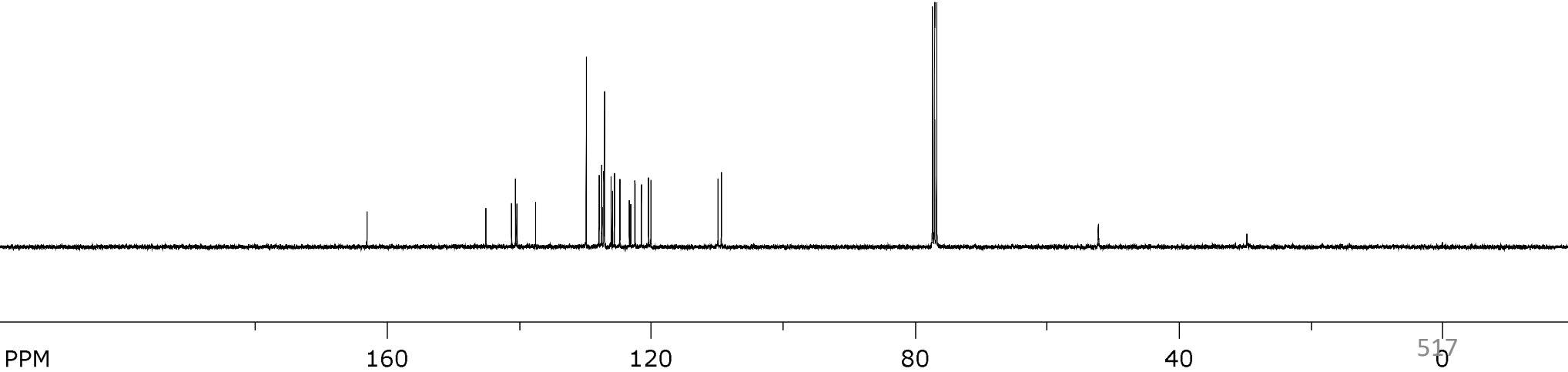
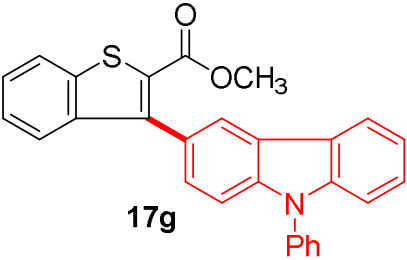
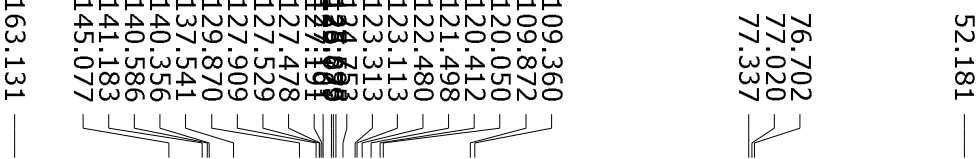
7.2996 —
7.3045 —

7.2890 —
7.2847 —
7.2804 —
7.2694 —
7.2648 —

7.2462 —

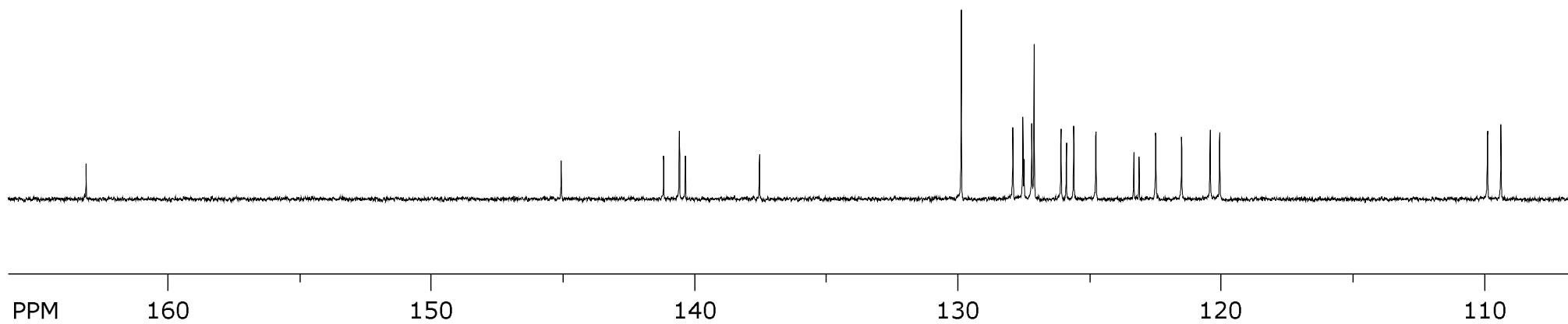
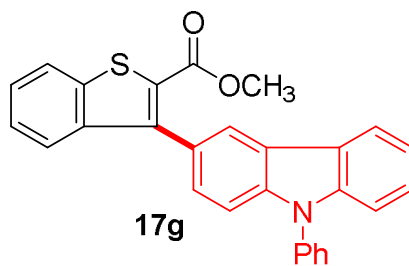


SpinWorks 4: RD 1266
C13CPD256 CDCl3 /opt/topspin3.5p12/nmrdata nmrsu 34

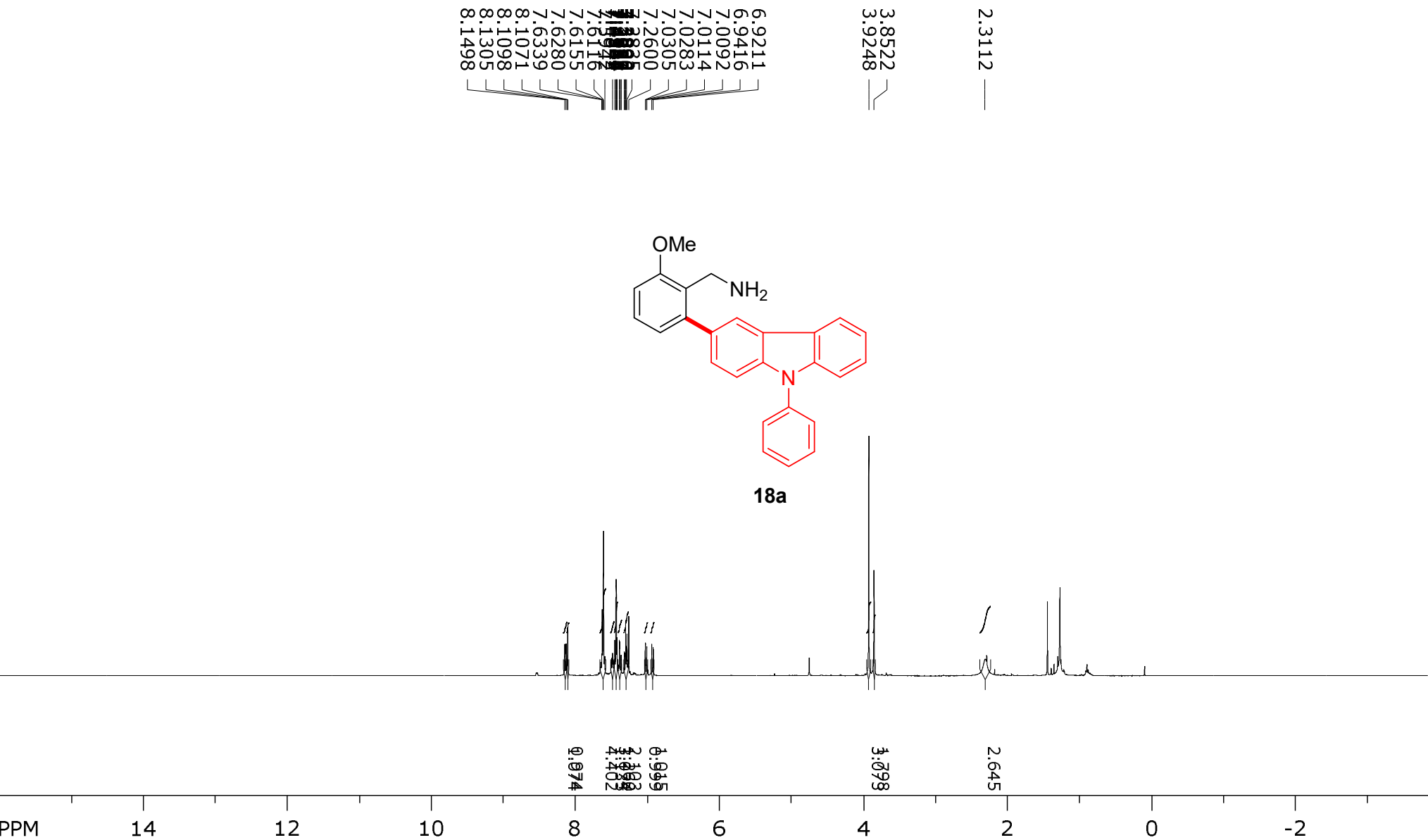


SpinWorks 4: RD 1266
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 34

163.131 —
145.077 —
140.356 —
140.586 —
141.183 —
137.541 —
129.870 —
127.909 —
127.529 —
127.478 —
127.191 —
127.101 —
126.079 —
125.875 —
125.595 —
124.753 —
123.313 —
123.113 —
122.480 —
121.498 —
120.412 —
120.050 —
109.872 —
109.360 —



SpinWorks 4: rd 1195
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

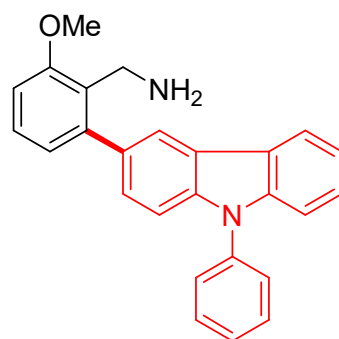


SpinWorks 4: rd 1195

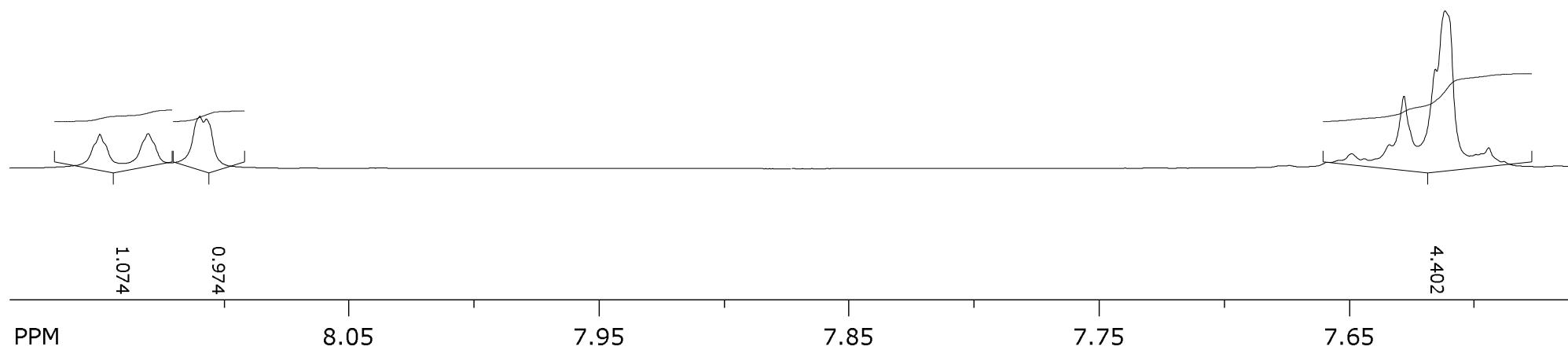
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

8.1071
8.1098
8.1305
8.1498

7.5942
7.6116
7.6155
7.6280
7.6339



18a



520

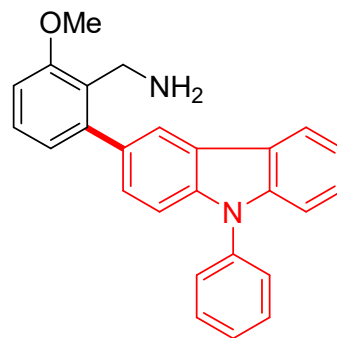
SpinWorks 4: rd 1195

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

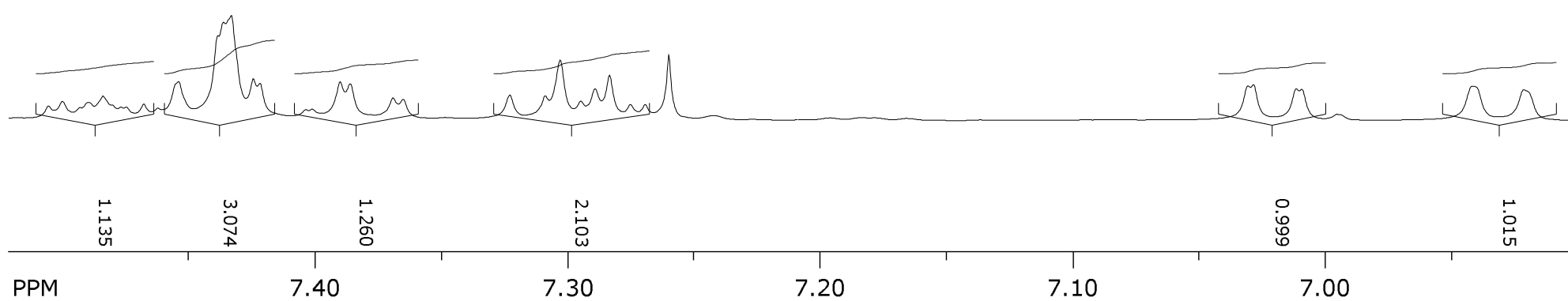
7.2600 —
7.2681 —
7.2747 —
7.2835 —
7.2892 —
7.3030 —
7.3090 —
7.3230 —
7.3652 —
7.3693 —
7.3862 —
7.3902 —
7.4006 —
7.4041 —
7.4220 —
7.4246 —
7.4334 —
7.4364 —
7.4387 —
7.4543 —
7.4684 —
7.4775 —
7.4842 —
7.4907 —
7.5004 —
7.5052 —

7.0092 —
7.0114 —
7.0283 —
7.0305 —

6.9211 —
6.9416 —



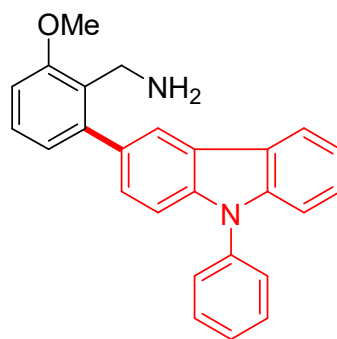
18a



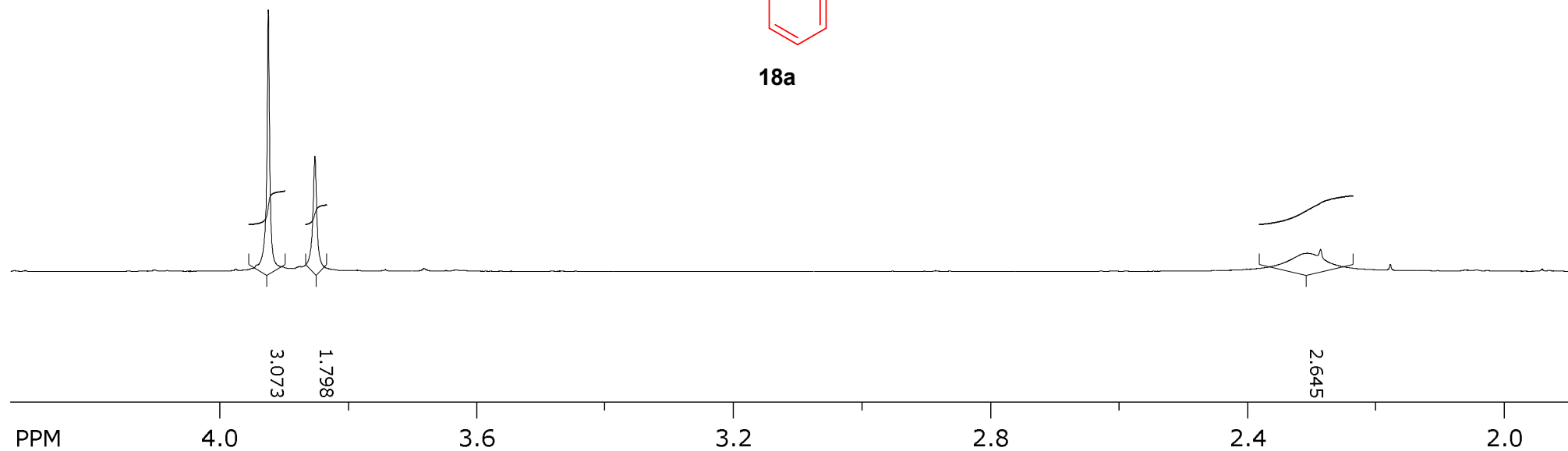
SpinWorks 4: rd 1195
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

3.9248
3.8522

2.3112

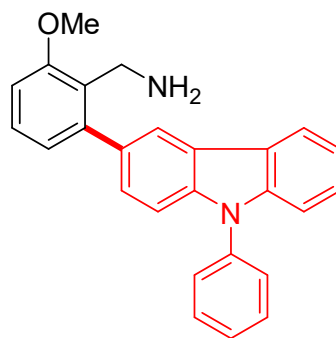
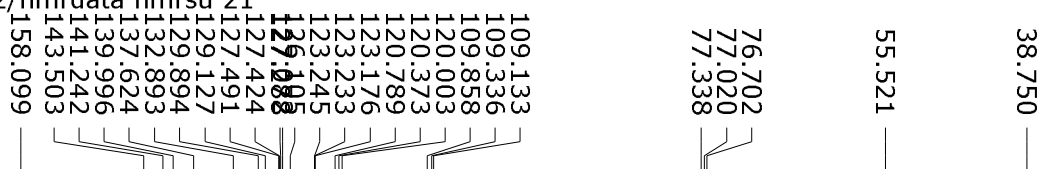


18a

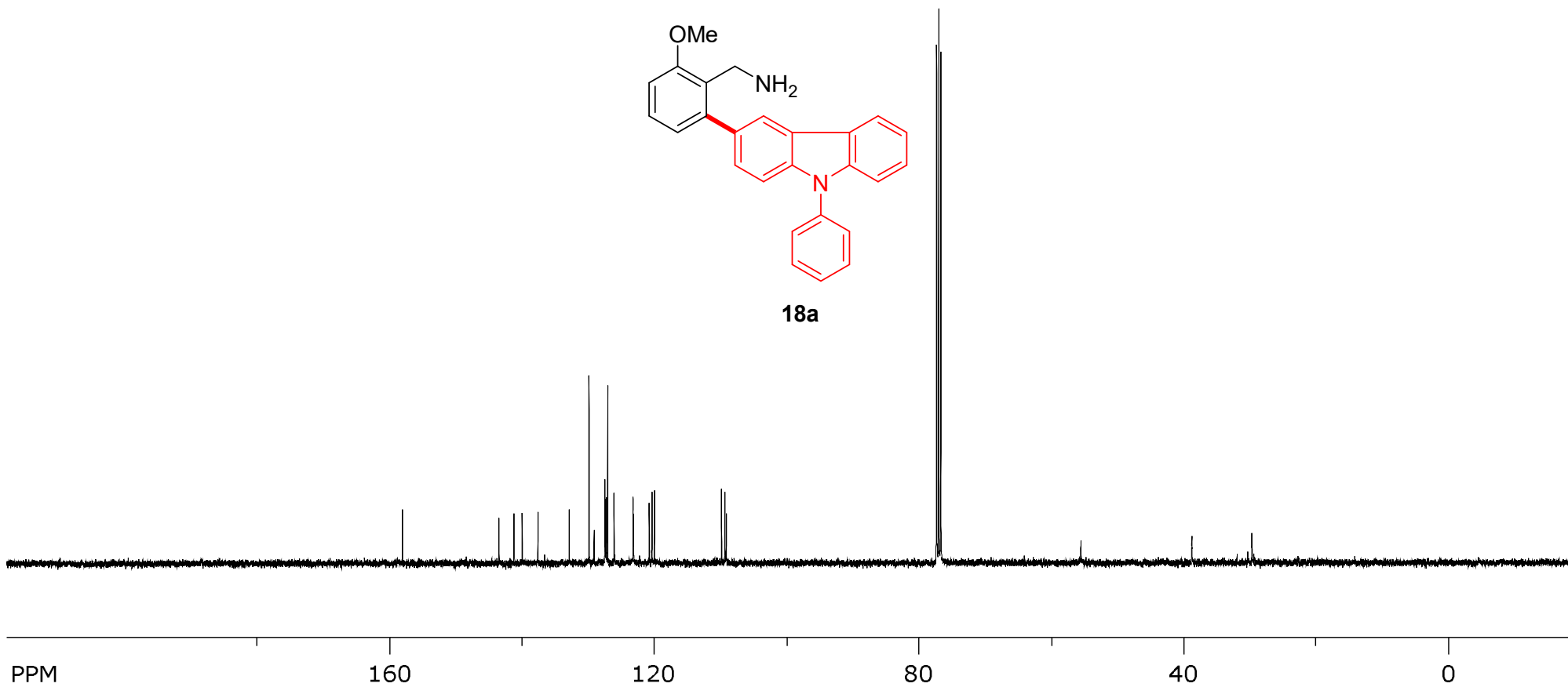


SpinWorks 4: rd 1195

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



18a



SpinWorks 4: rd 1195

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

158.099

143.503

141.242

139.996

137.624

132.893

129.894

129.127

127.491

127.424

127.288

127.072

126.105

123.245

123.233

123.176

120.789

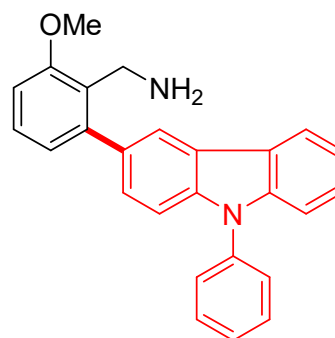
120.373

120.003

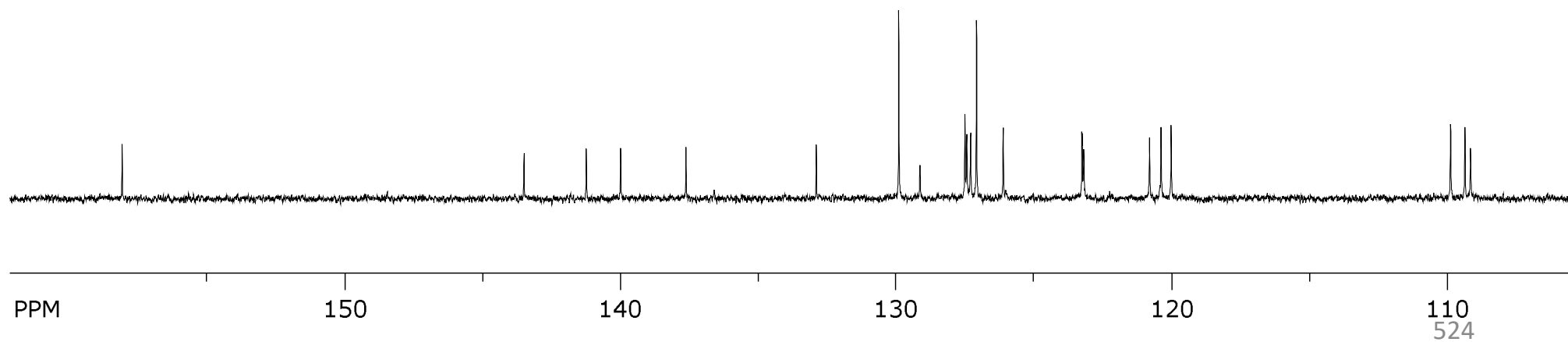
109.858

109.336

109.133



18a



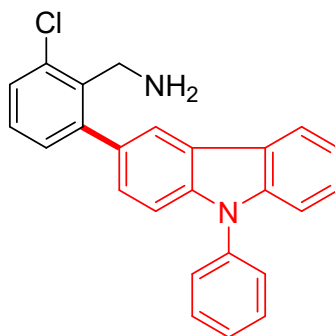
SpinWorks 4: RD-2028

PROTON CDCl₃ /opt/topspin3.5pl2/nmrdata nmrsu 12

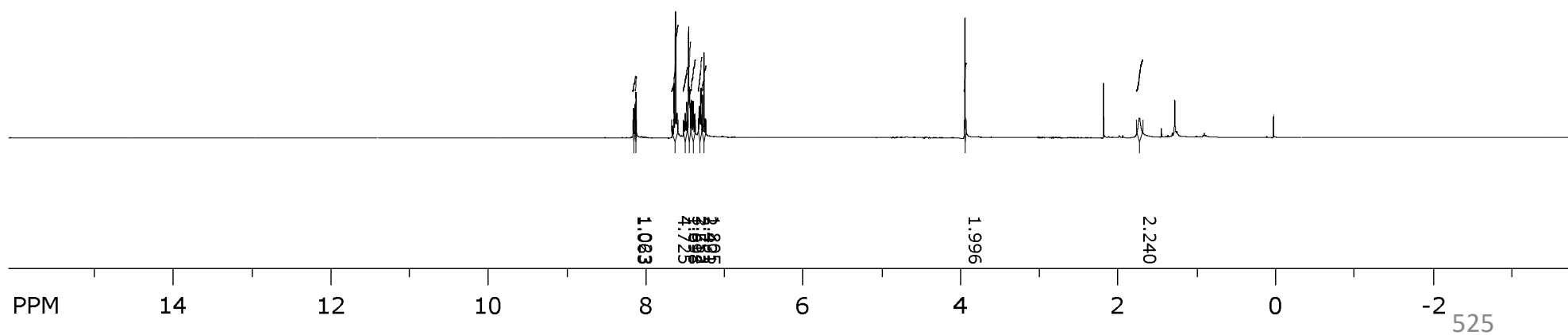
7.2410
7.2600
7.2792
7.2909
7.2981
7.3021
7.3108
7.3140
7.3140
7.3140
7.6411
7.6462
7.6618
8.1239
8.1271
8.1358
8.1552

3.9445

1.7280



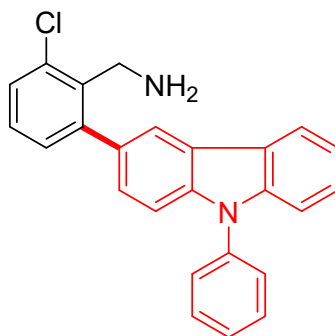
18b



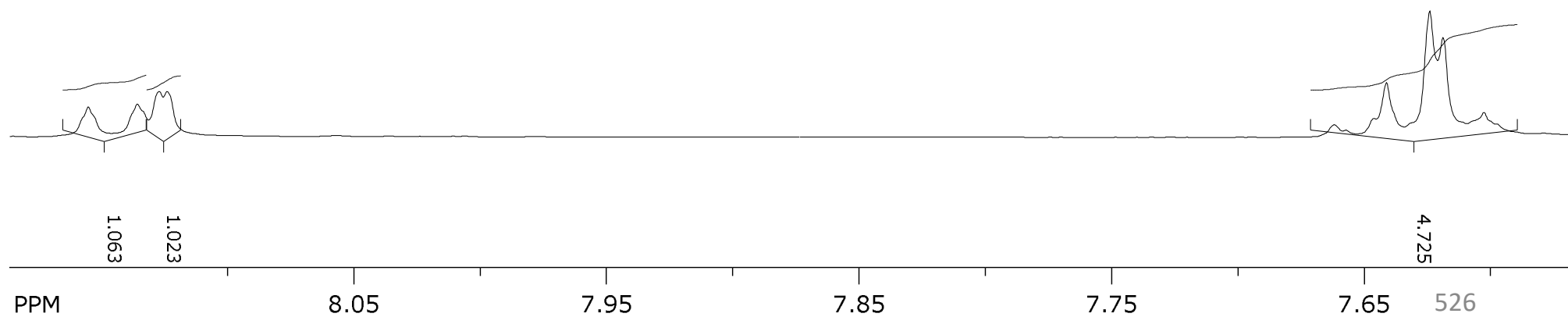
SpinWorks 4: RD-2028
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

8.1239
8.1271
8.1358
8.1552

7.5975
7.6025
7.6187
7.6240
7.6411
7.6462
7.6618

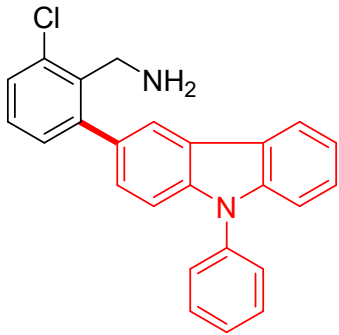


18b

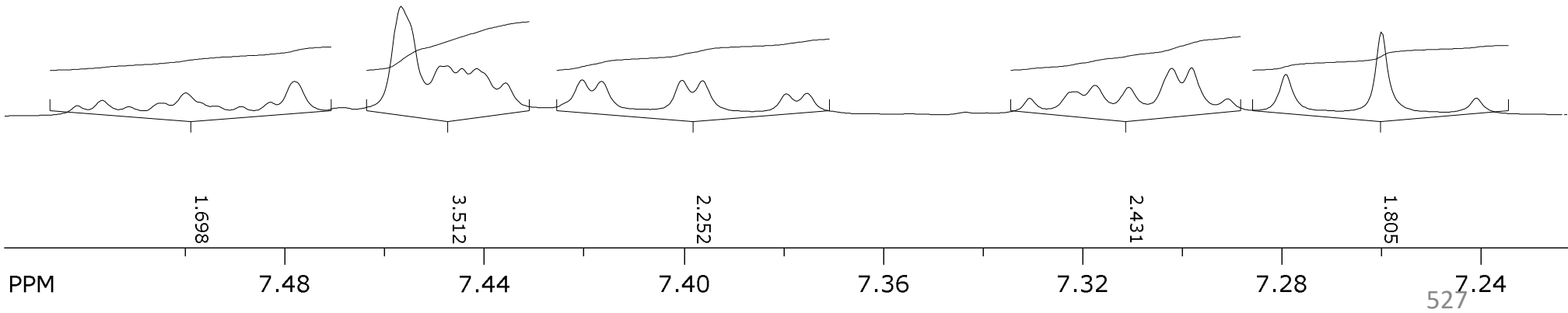


SpinWorks 4: RD-2028
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

7.2410 —
7.2600 —
7.2792 —
7.2909 —
7.2981 —
7.3021 —
7.3108 —
7.3175 —
7.3215 —
7.3306 —
7.3753 —
7.3794 —
7.3962 —
7.4004 —
7.4165 —
7.4205 —
7.4358 —
7.4416 —
7.4446 —
7.4475 —
7.4488 —
7.4568 —
7.4782 —
7.4831 —
7.4889 —
7.4939 —
7.5000 —
7.5046 —
7.5114 —
7.5168 —
7.5217 —



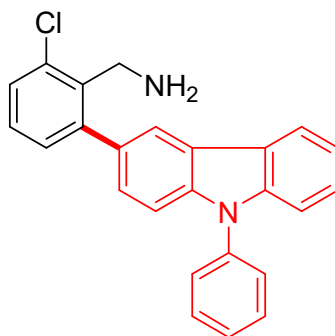
18b



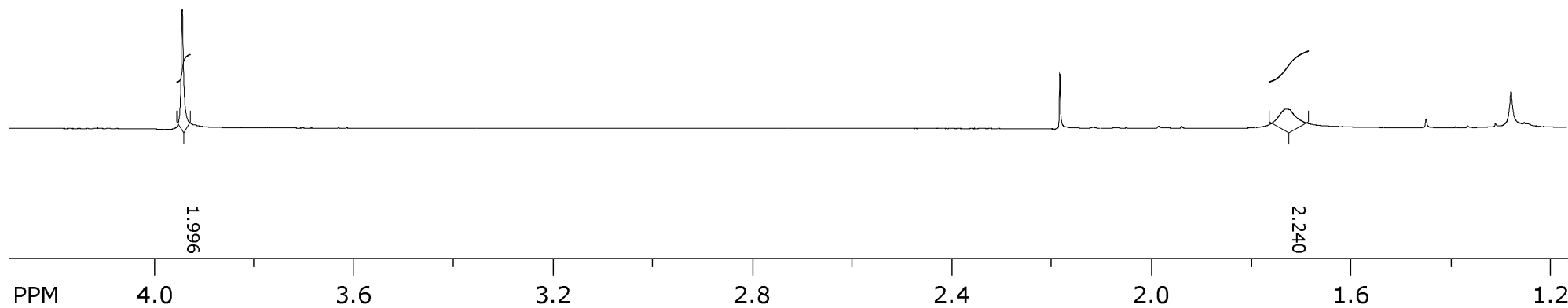
SpinWorks 4: RD-2028
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

3.9445

1.7280



18b



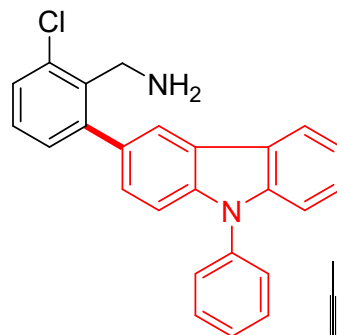
SpinWorks 4: RD-2028

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

109.474
109.931
120.111
120.346
120.710
123.088
123.267
126.266
127.006
127.987
128.805
129.537
129.925
132.423
134.808
137.481
138.759
140.125
141.279
144.546

76.702
77.020
77.338

41.562



18b

PPM

160

120

80

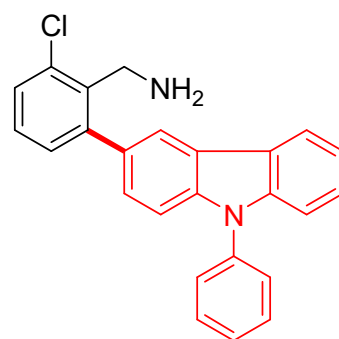
40

0

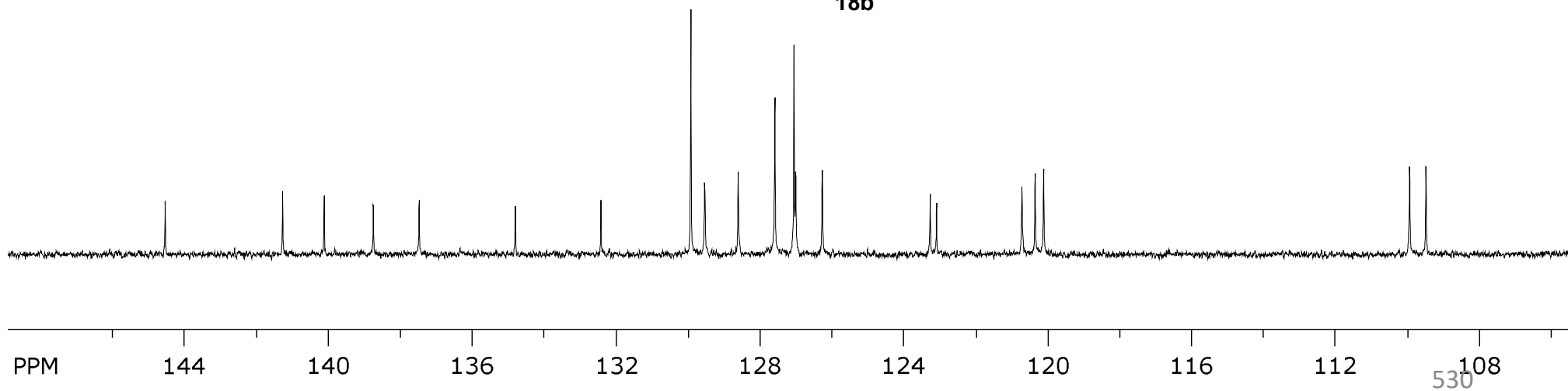
SpinWorks 4: RD-2028

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

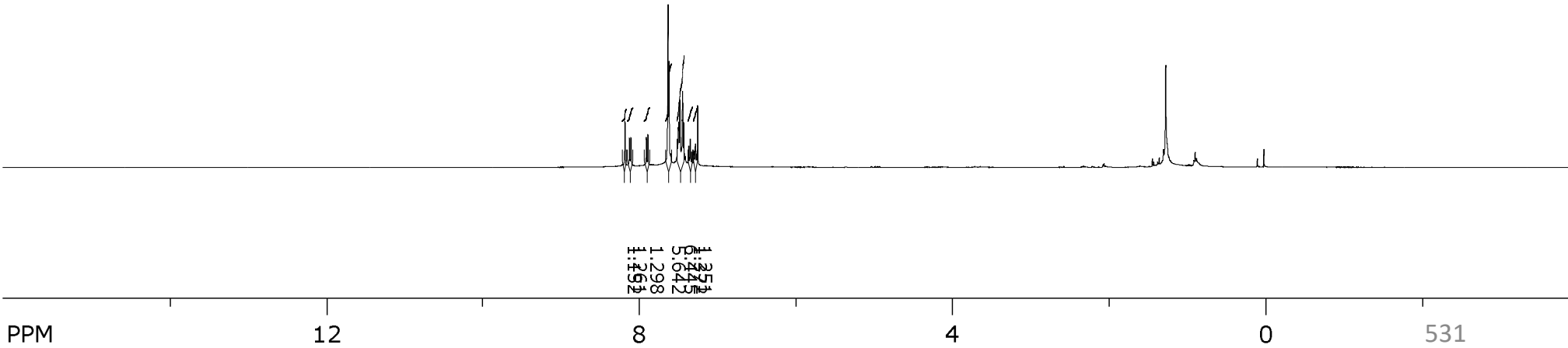
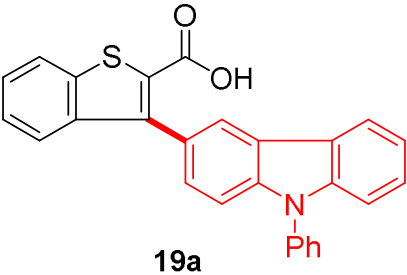
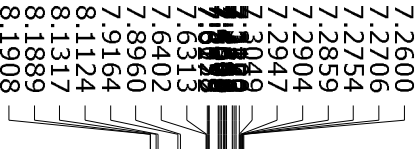
144.546 —
141.279 —
140.125 —
138.759 —
137.481 —
134.808 —
132.423 —
129.925 —
129.537 —
128.605 —
127.587 —
127.057 —
127.006 —
126.266 —
123.267 —
123.088 —
120.710 —
120.346 —
120.111 —
109.474 —
109.931 —



18b



SpinWorks 4: RD-2055
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



SpinWorks 4: RD-2055

PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

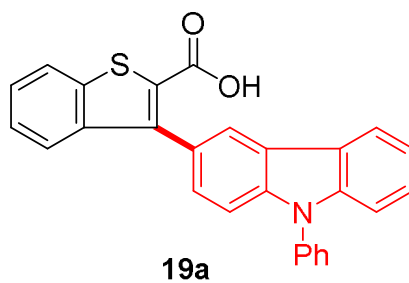
8.1908

8.1317

8.1124

7.9164

7.8960



19a

1.152

1.261

1.298

532
7.88

PPM

8.20

8.16

8.12

8.08

8.04

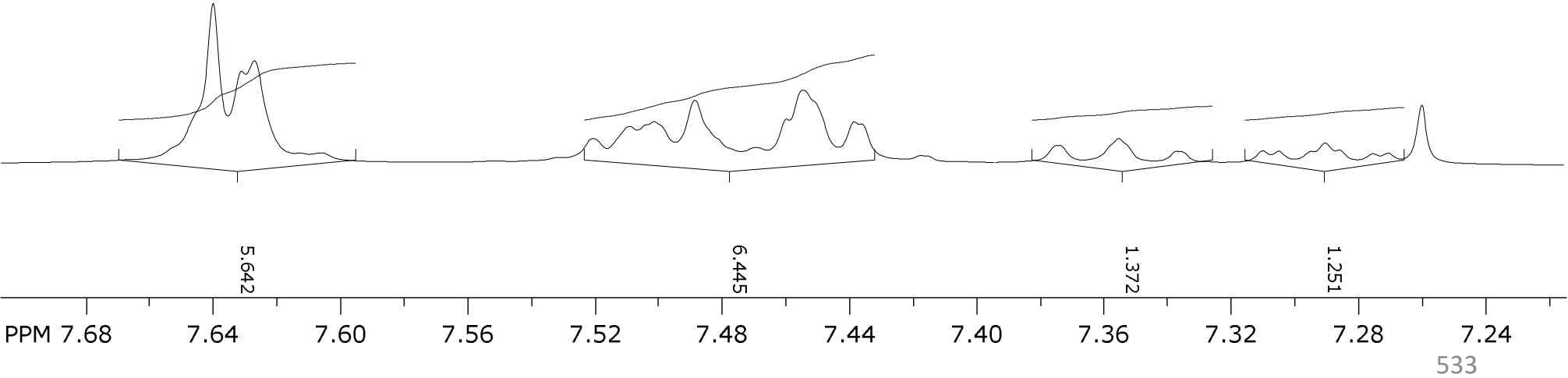
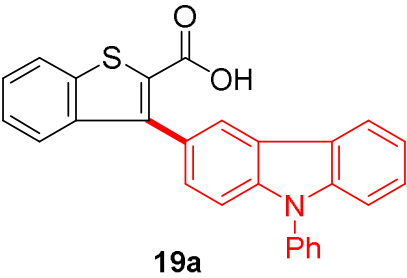
8.00

7.96

7.92

SpinWorks 4: RD-2055
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

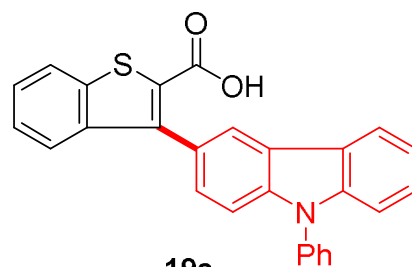
7.6272	7.6059	7.5205	7.4887	7.4547	7.4386	7.3743	7.3553	7.3370	7.3100	7.2947	7.2706	7.2600
7.6313	7.6128	7.5092	7.5015	7.4598	7.4362	7.3747					7.2754	
7.6402											7.2859	
											7.2904	
											7.3049	
											7.3100	



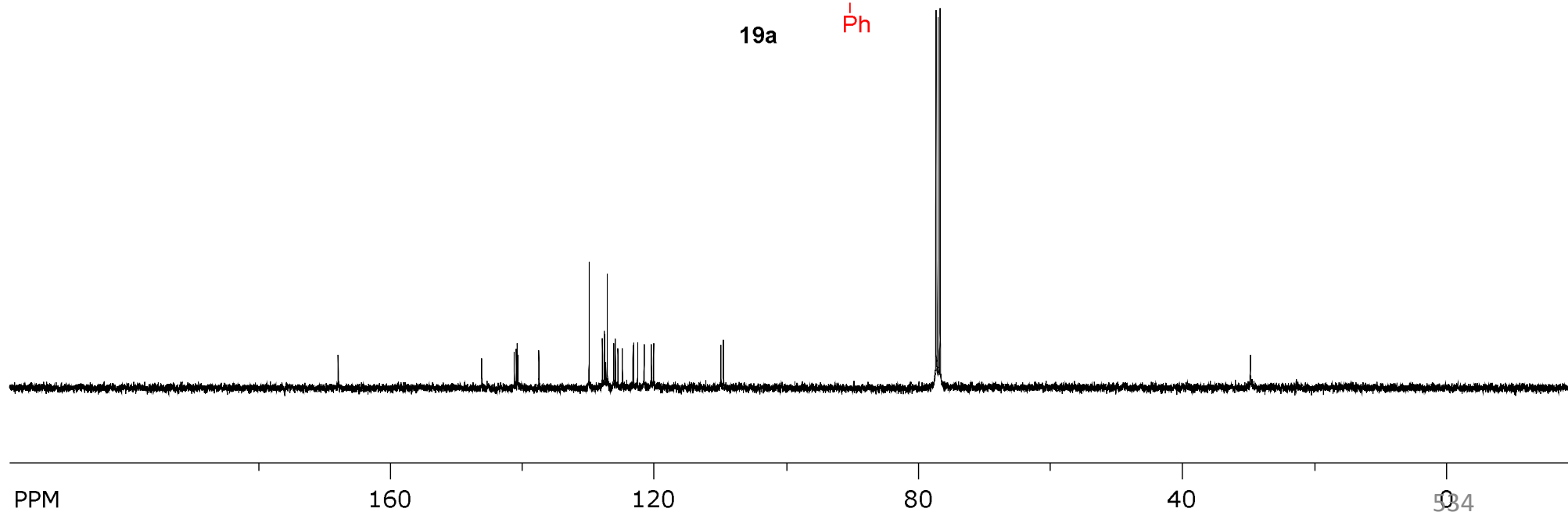
SpinWorks 4: RD-2055

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

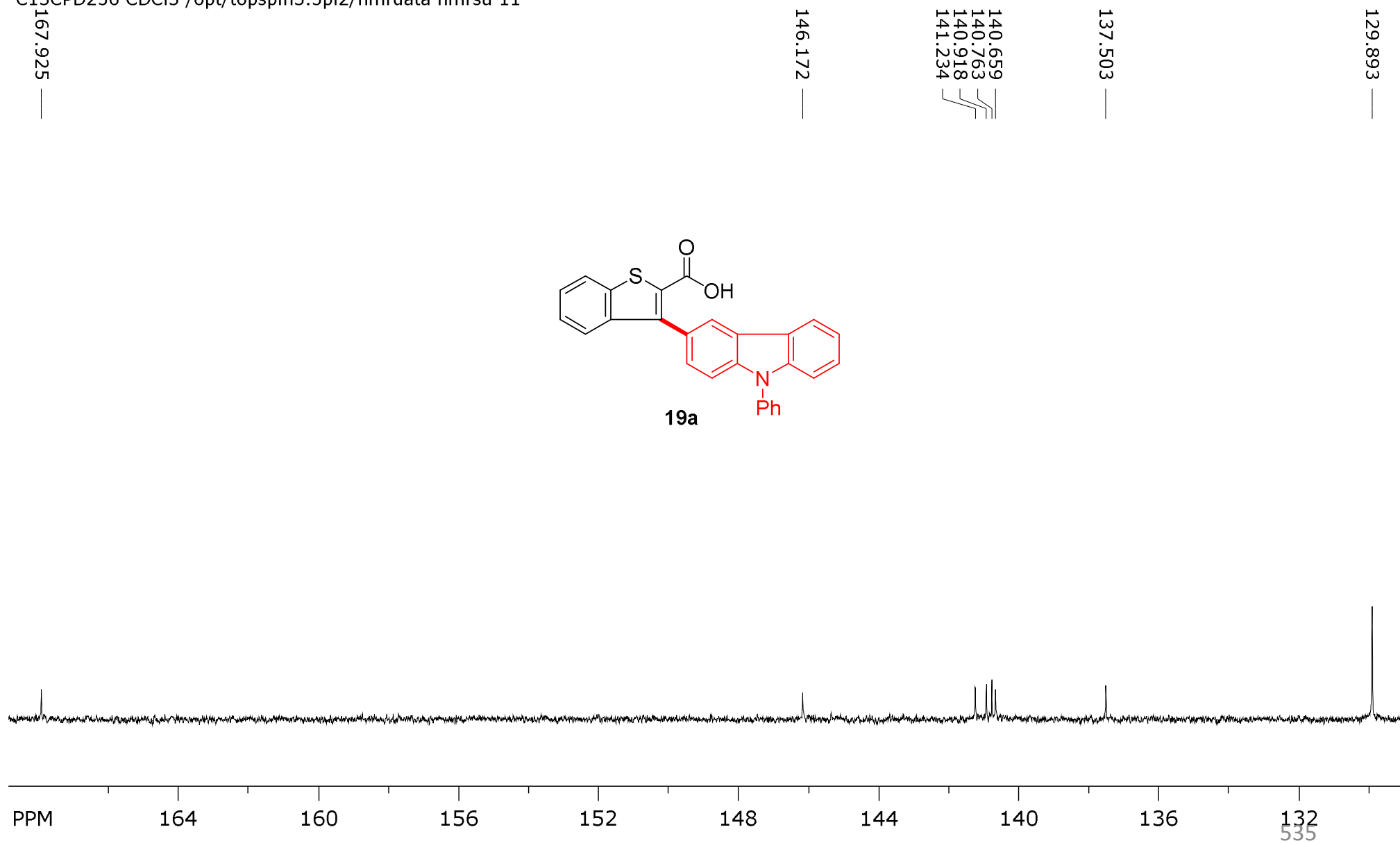
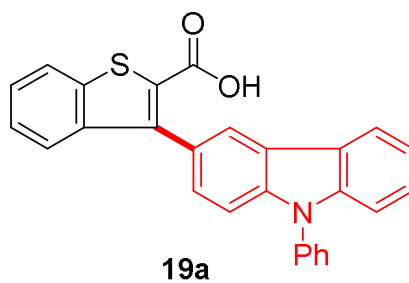
167.925
146.172
141.234
140.918
140.763
140.659
137.503
129.893
127.874
127.569
127.531
127.129
124.969
124.968
123.236
123.155
122.525
121.552
120.450
120.125
109.917
109.540
76.702
77.020
77.337



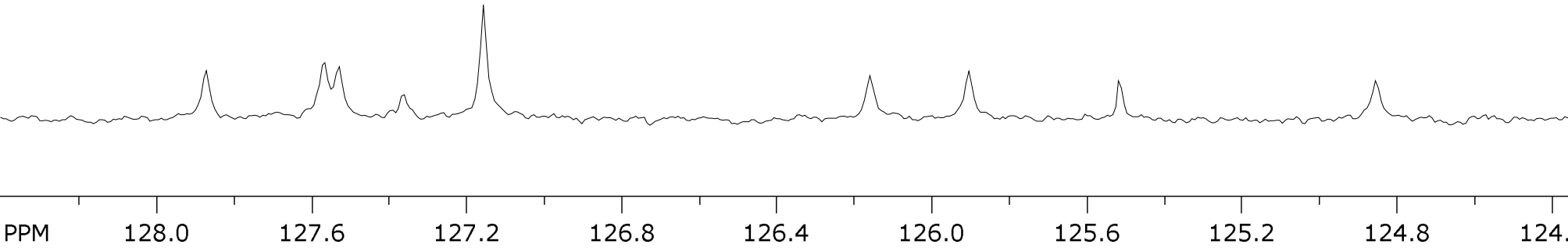
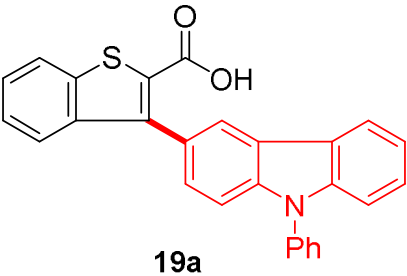
19a



SpinWorks 4: RD-2055
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



SpinWorks 4: RD-2055
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



SpinWorks 4: RD-2055

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

123.155
123.236

122.525

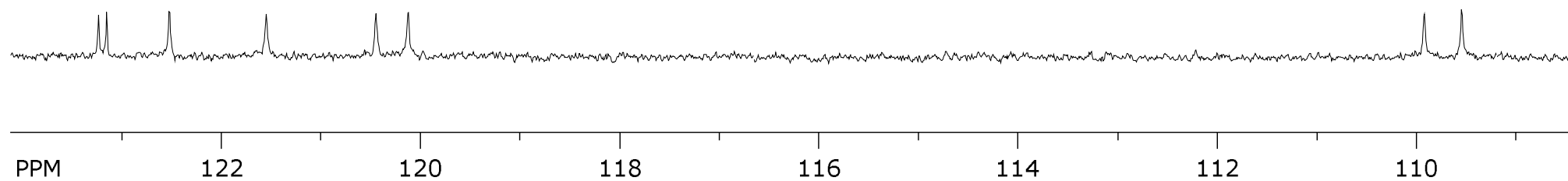
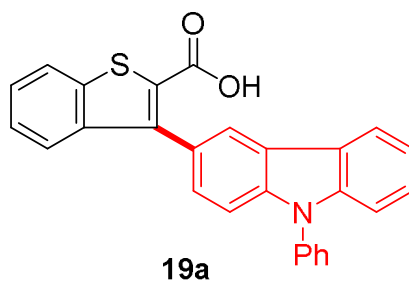
121.552

120.450

120.125

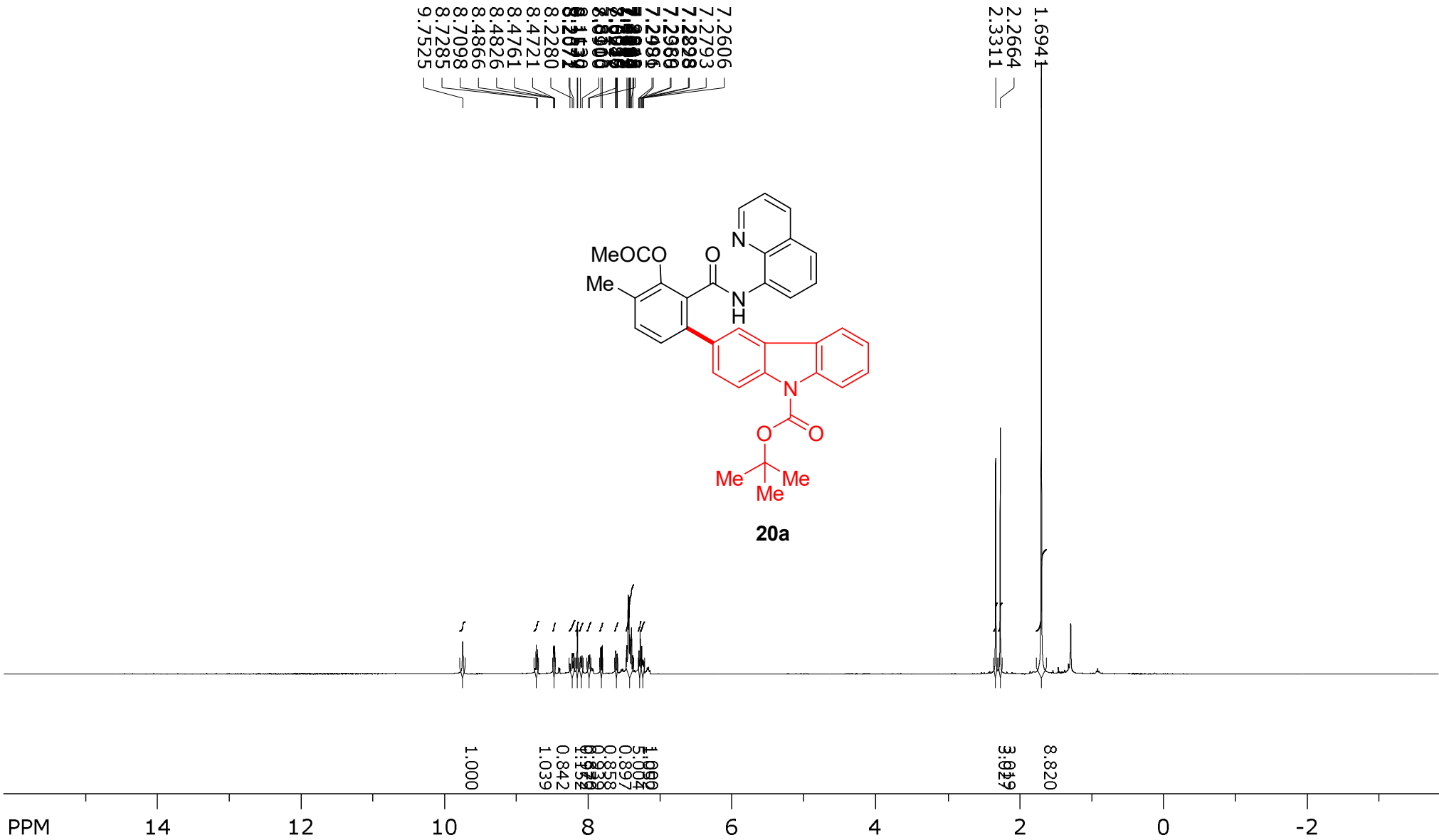
109.917

109.540

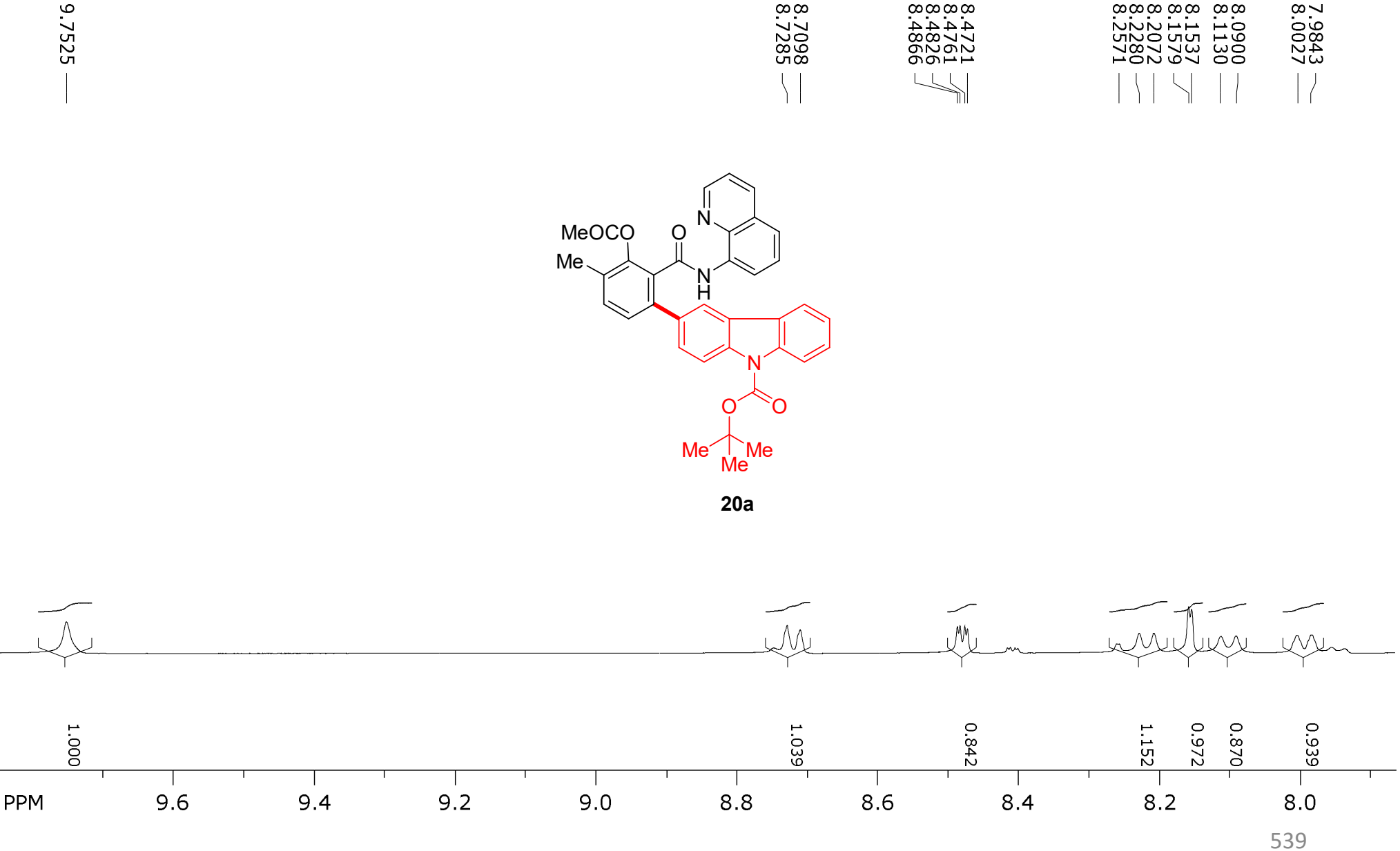


537

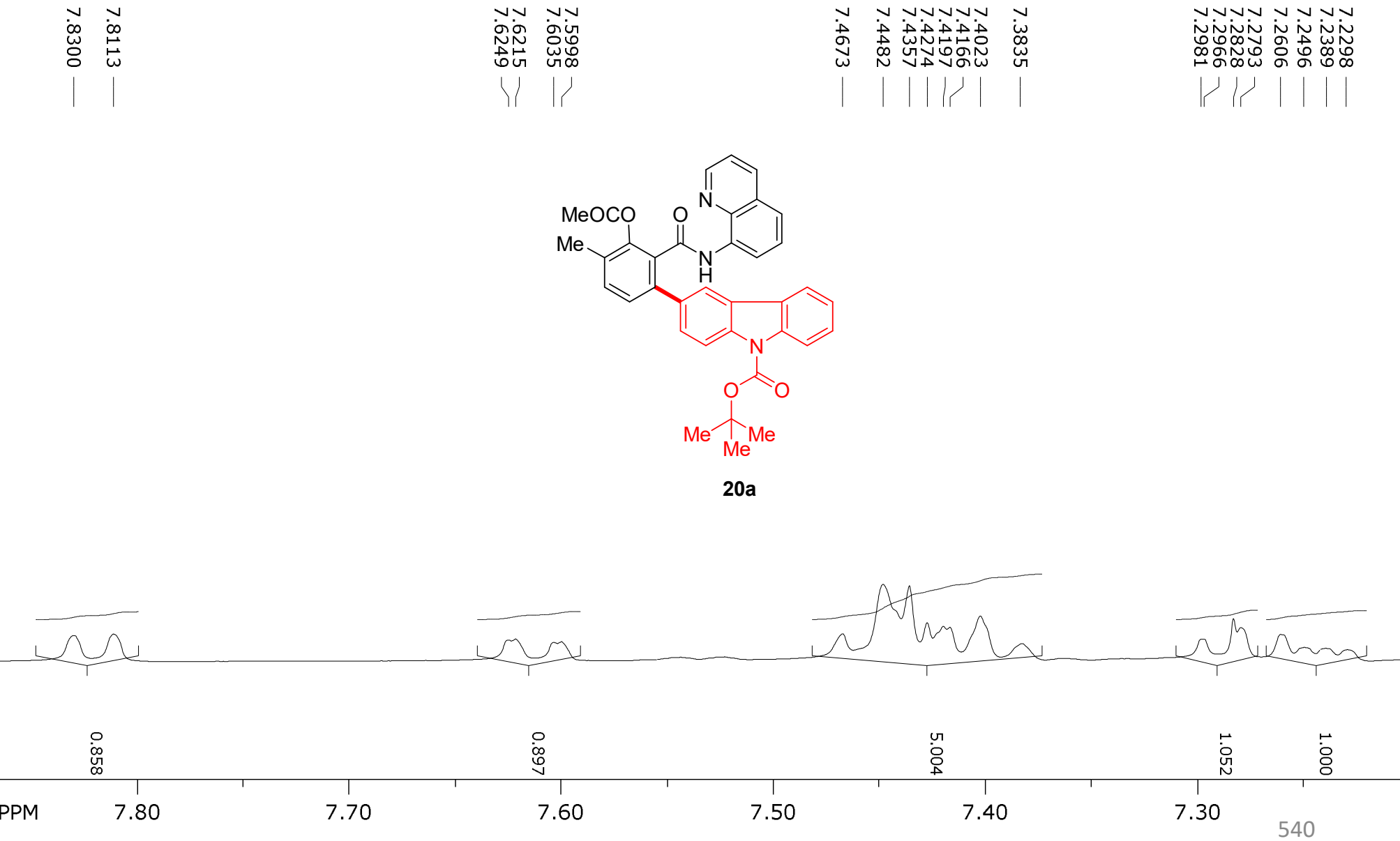
SpinWorks 4: RD 1246
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: RD 1246
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

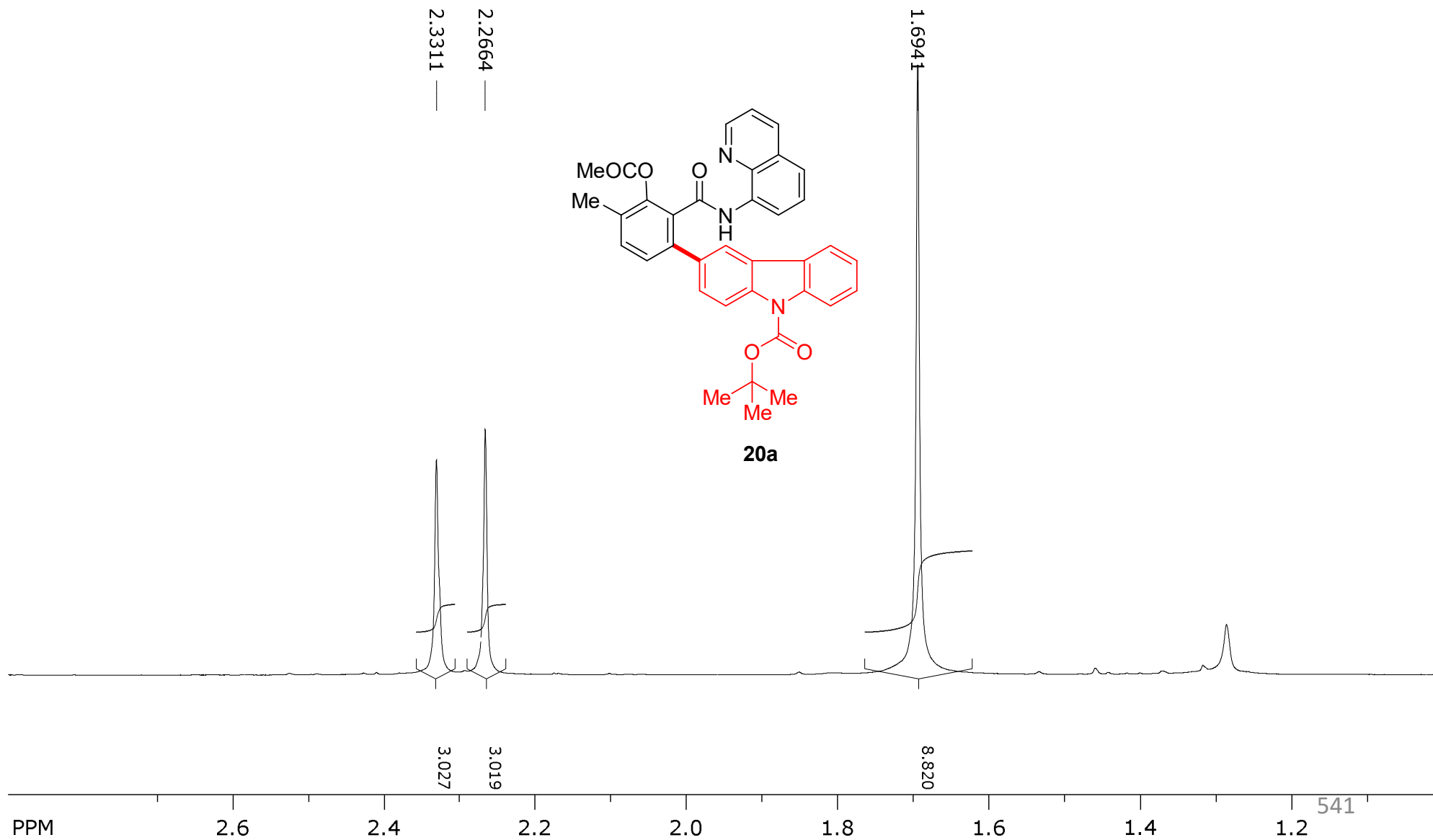
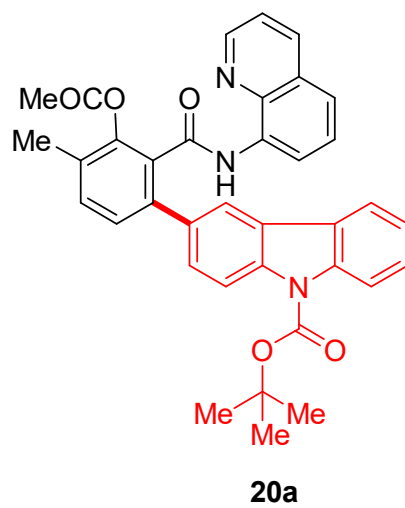


SpinWorks 4: RD 1246
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



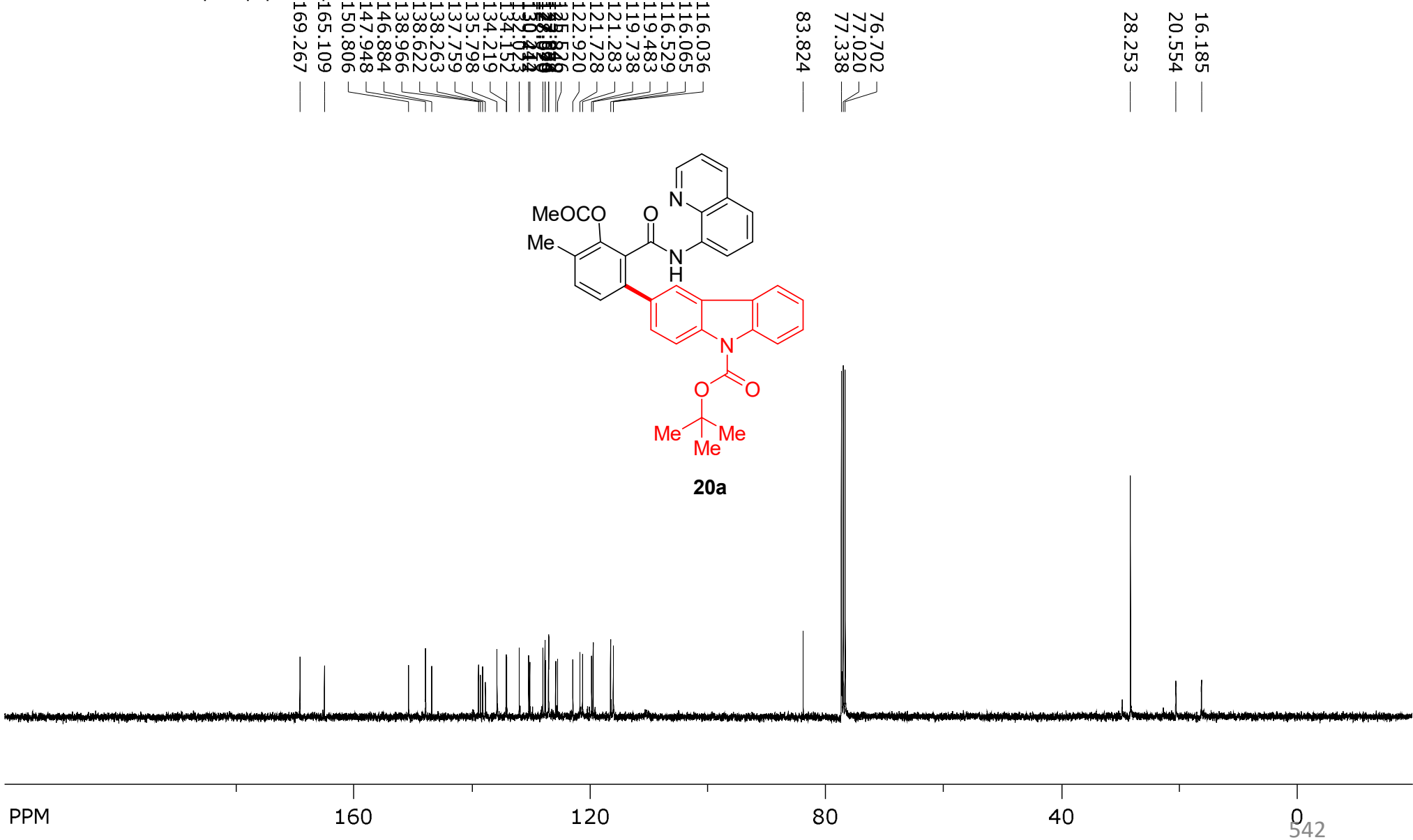
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

2.2664 —
2.3311 —



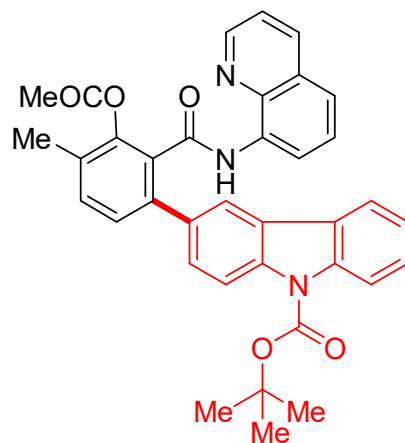
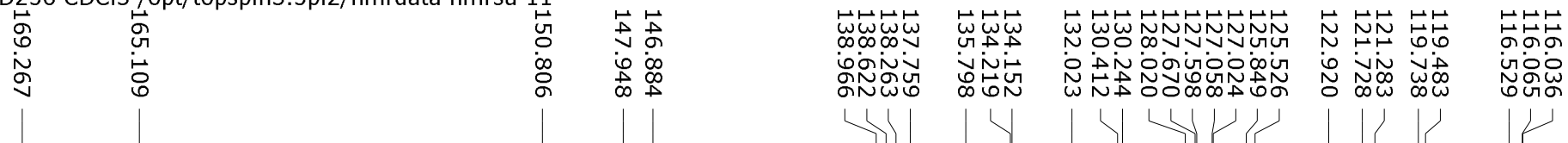
SpinWorks 4: RD-1246

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

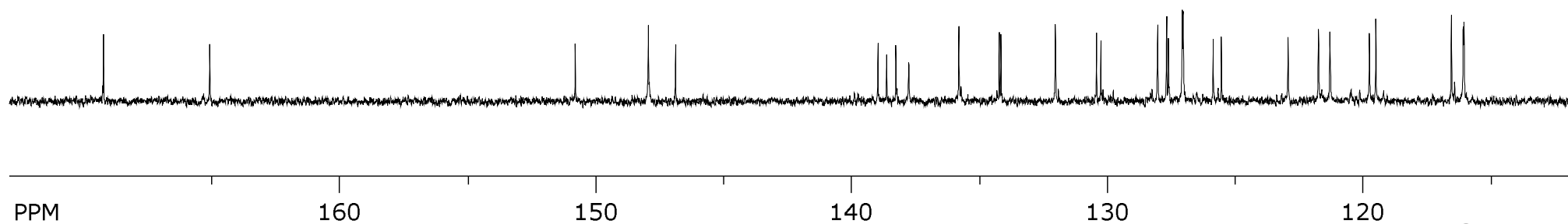


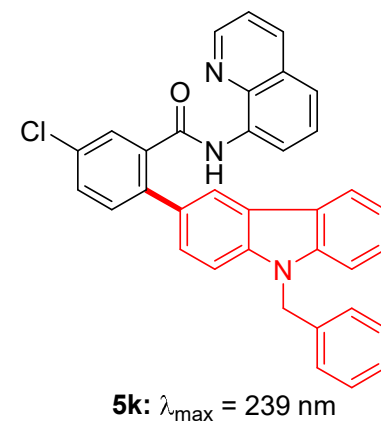
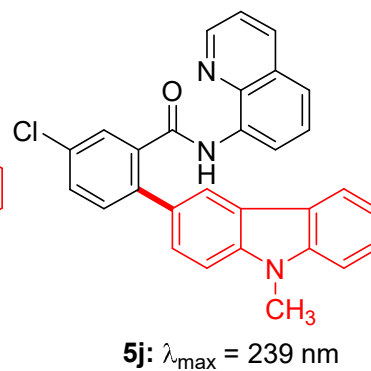
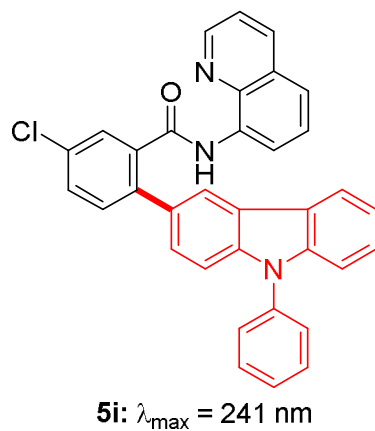
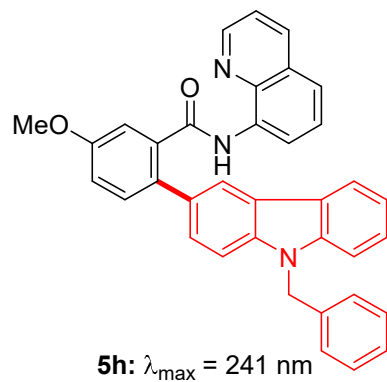
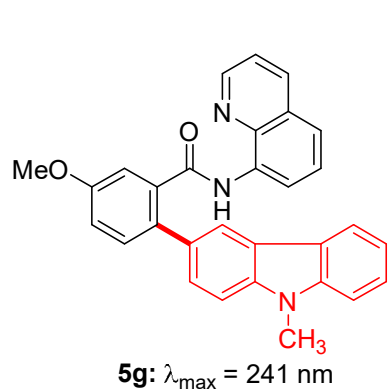
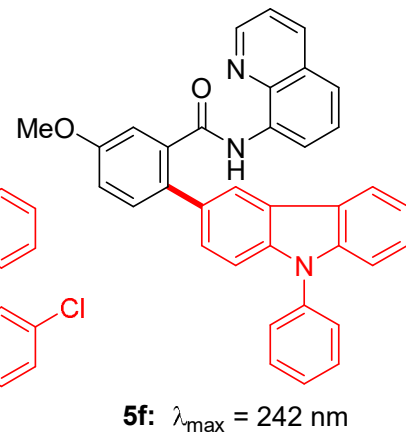
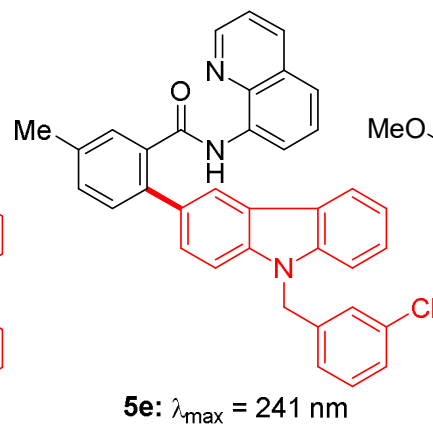
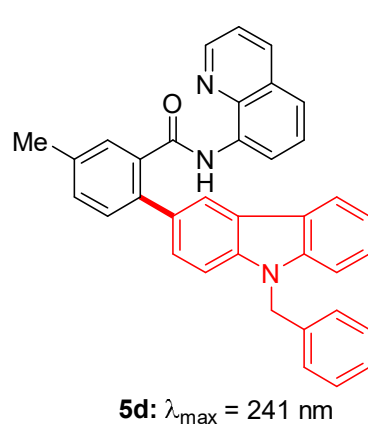
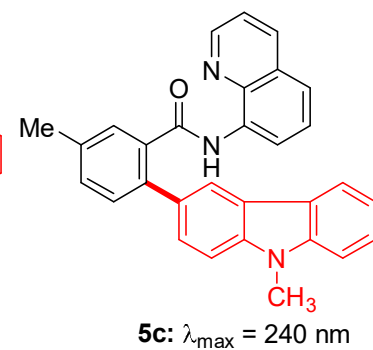
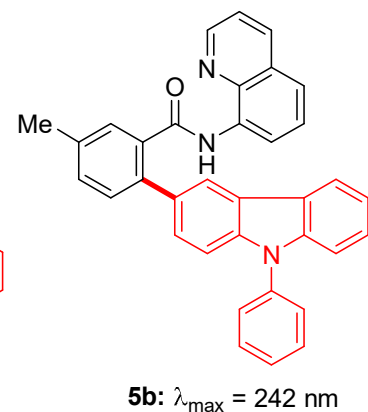
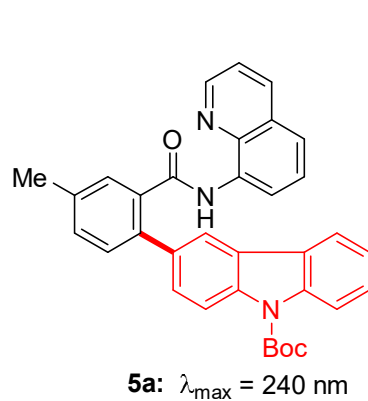
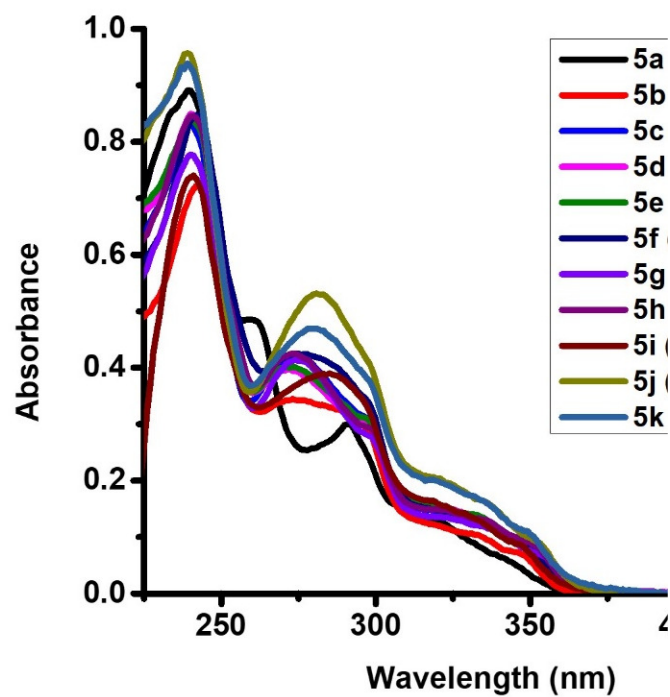
SpinWorks 4: RD-1246

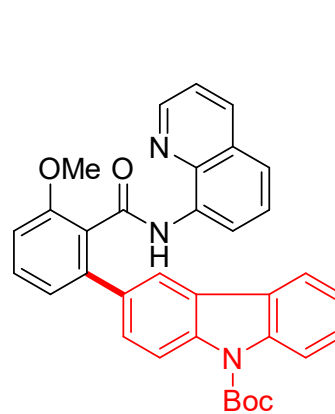
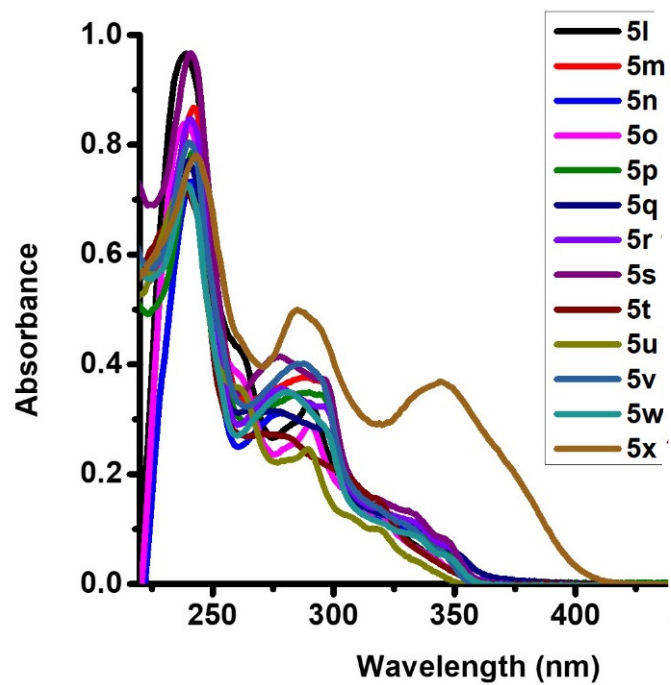
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



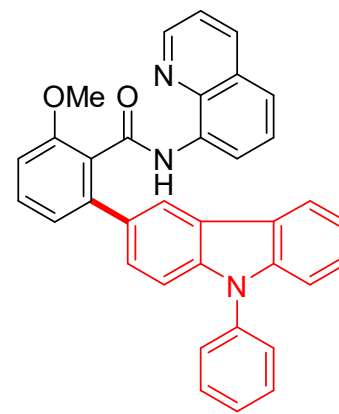
20a



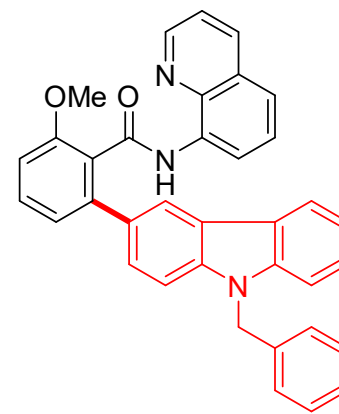




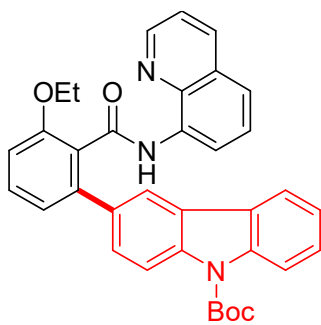
5l: $\lambda_{\text{max}} = 239 \text{ nm}$



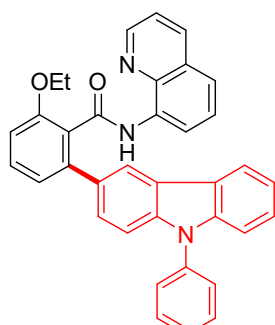
5m: $\lambda_{\text{max}} = 243 \text{ nm}$



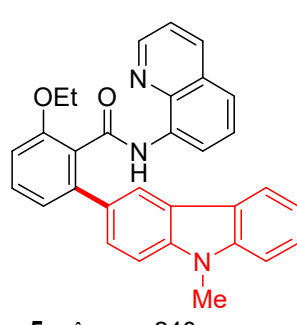
5n: $\lambda_{\text{max}} = 241 \text{ nm}$



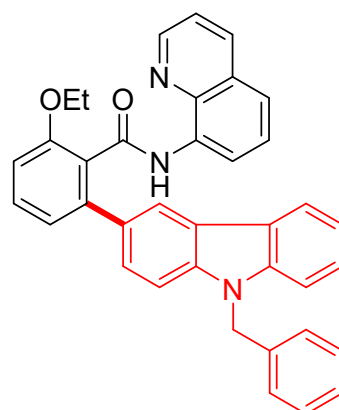
5o: $\lambda_{\text{max}} = 238 \text{ nm}$



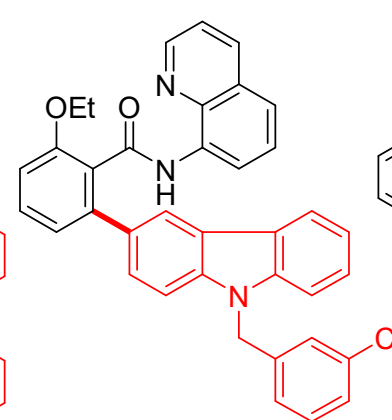
5p: $\lambda_{\text{max}} = 243 \text{ nm}$



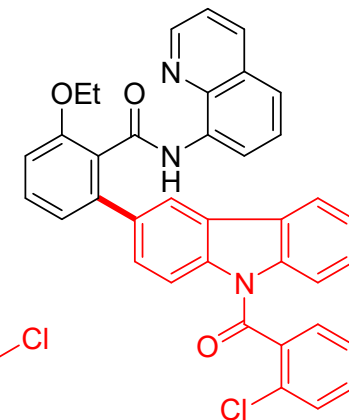
5q: $\lambda_{\text{max}} = 240 \text{ nm}$



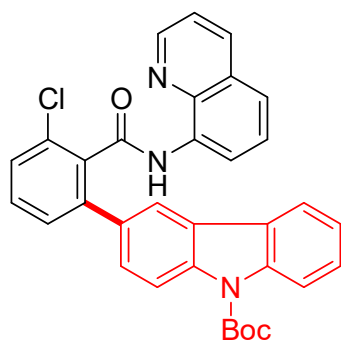
5r: $\lambda_{\text{max}} = 241 \text{ nm}$



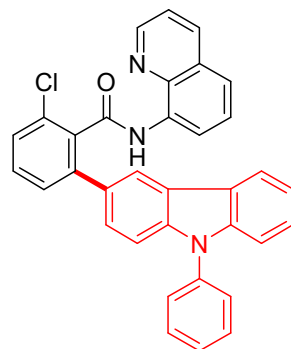
5s: $\lambda_{\text{max}} = 240 \text{ nm}$



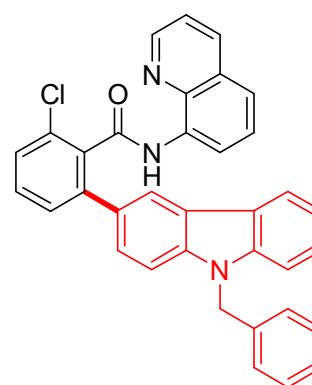
5t: $\lambda_{\text{max}} = 240 \text{ nm}$



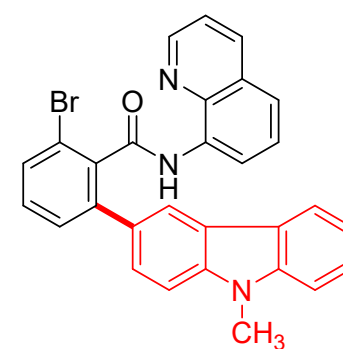
5u: $\lambda_{\text{max}} = 240 \text{ nm}$



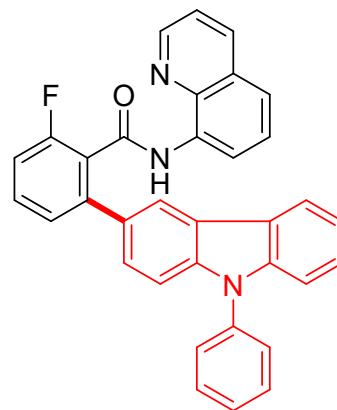
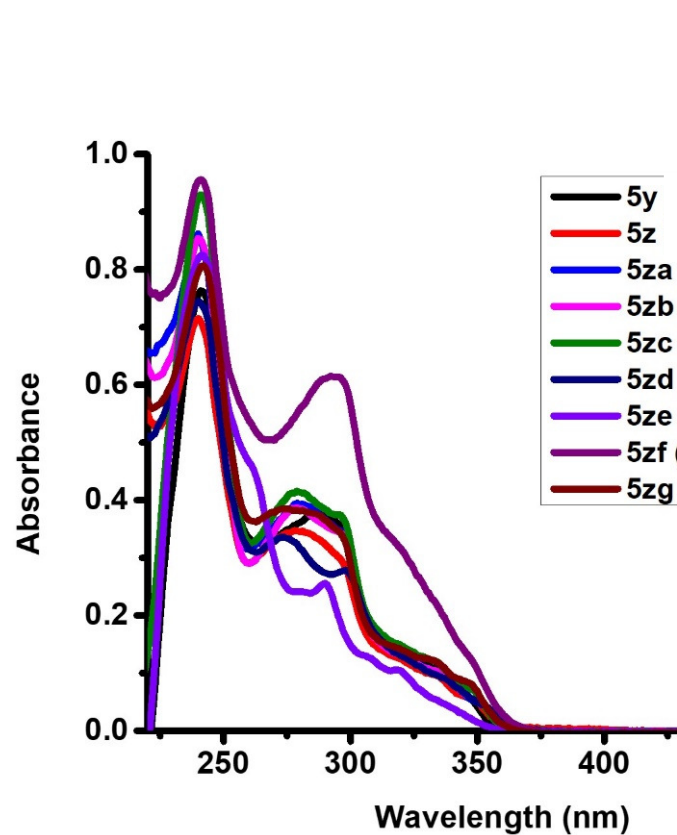
5v: $\lambda_{\text{max}} = 240 \text{ nm}$



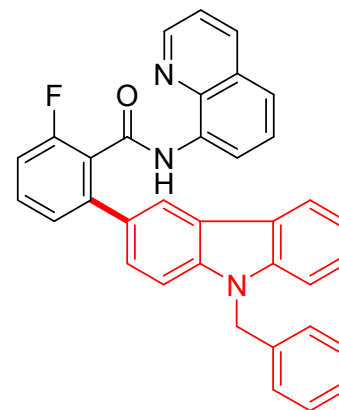
5w: $\lambda_{\text{max}} = 239 \text{ nm}$



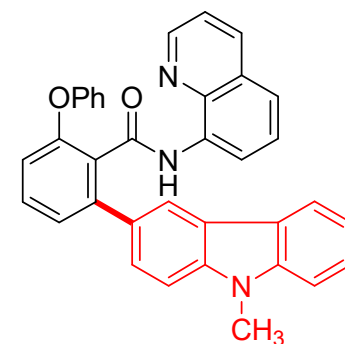
5x: $\lambda_{\text{max}} = 243 \text{ nm}$



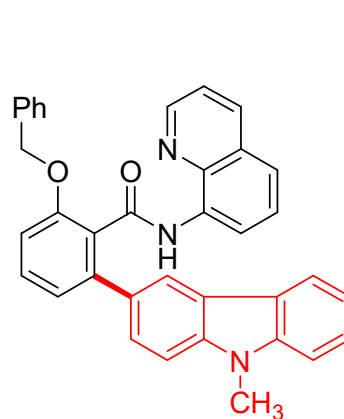
5y: $\lambda_{\text{max}} = 241 \text{ nm}$



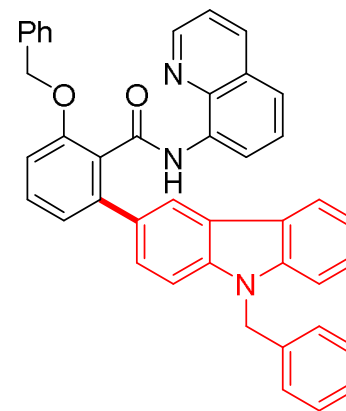
5z: $\lambda_{\text{max}} = 240 \text{ nm}$



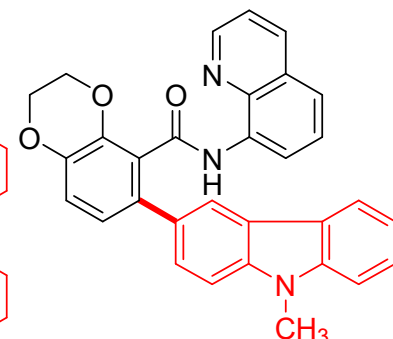
5za: $\lambda_{\text{max}} = 248 \text{ nm}$



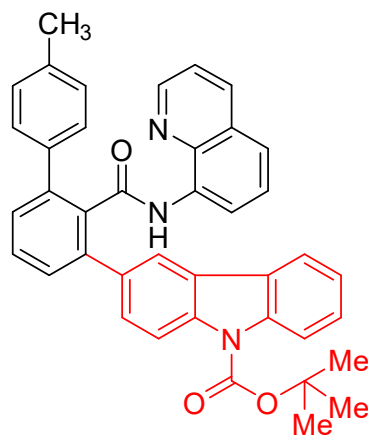
5zb: $\lambda_{\text{max}} = 241 \text{ nm}$



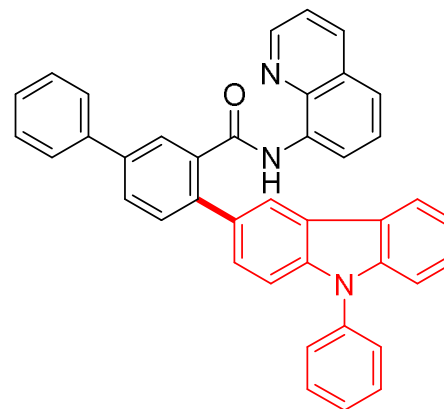
5zc: $\lambda_{\text{max}} = 242 \text{ nm}$



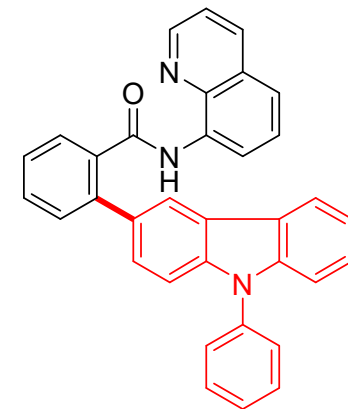
5zd: $\lambda_{\text{max}} = 240 \text{ nm}$



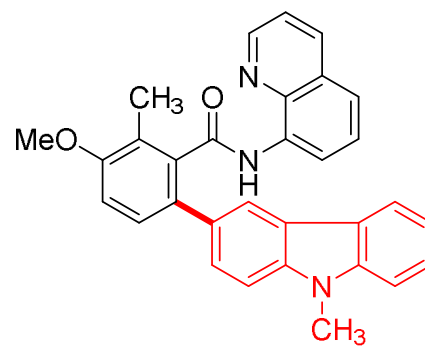
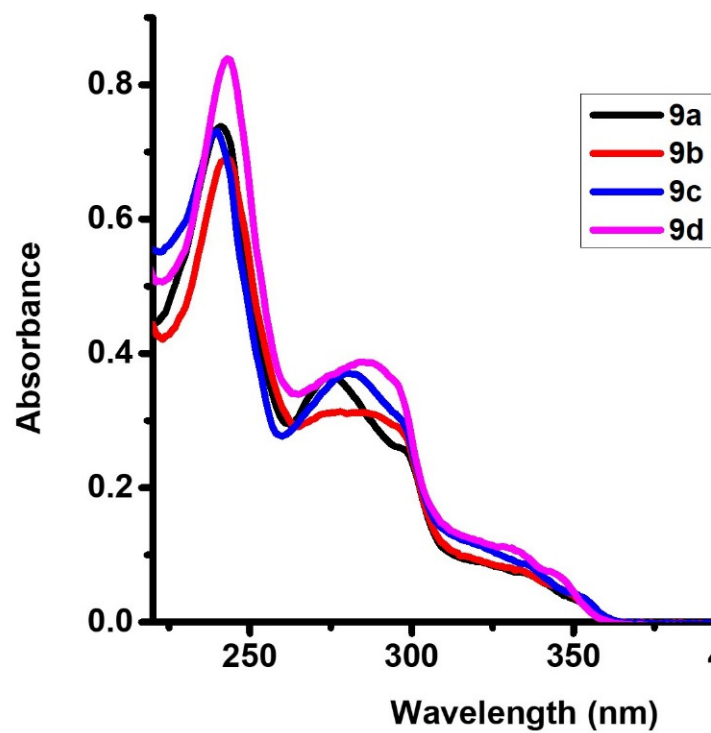
5ze: $\lambda_{\text{max}} = 242 \text{ nm}$



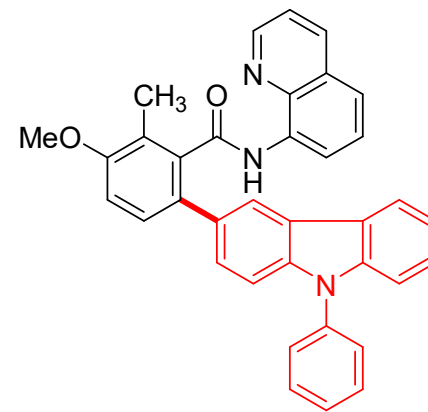
5zf: $\lambda_{\text{max}} = 242 \text{ nm}$



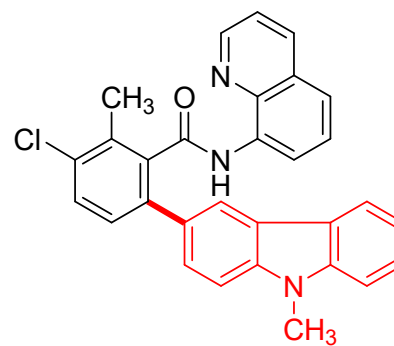
5zg: $\lambda_{\text{max}} = 242 \text{ nm}$



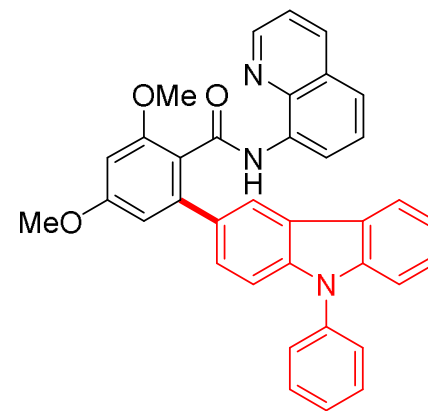
9a: $\lambda_{\text{max}} = 242 \text{ nm}$



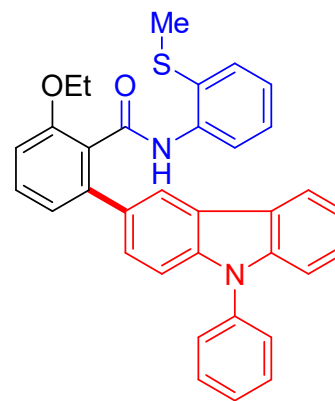
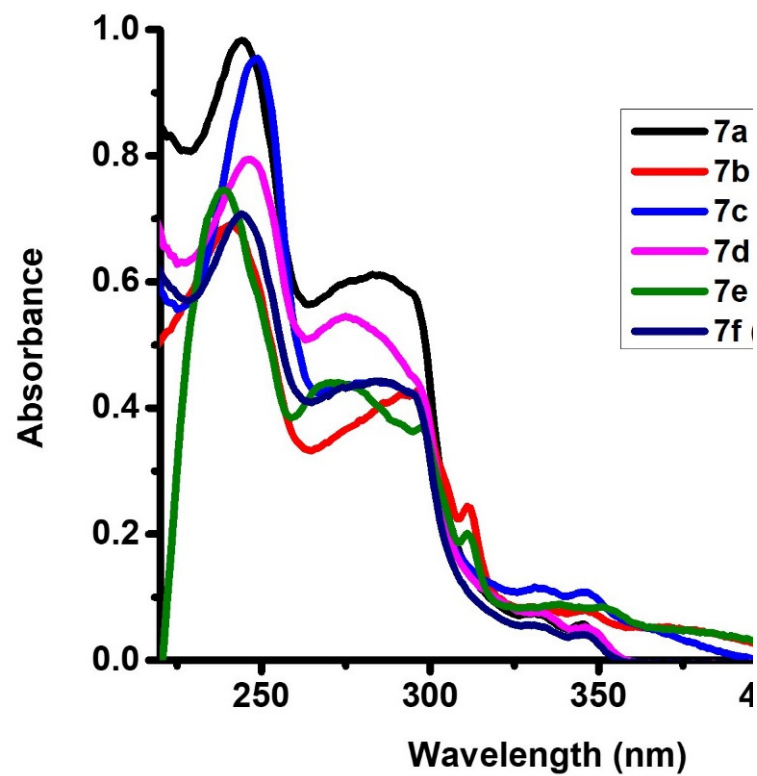
9b: $\lambda_{\text{max}} = 242 \text{ nm}$



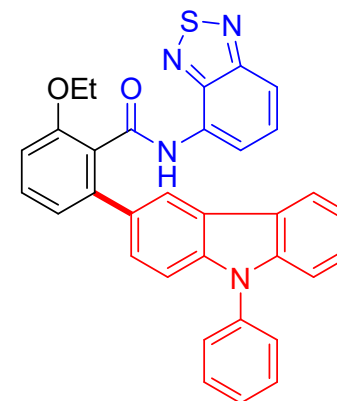
9c: $\lambda_{\text{max}} = 240 \text{ nm}$



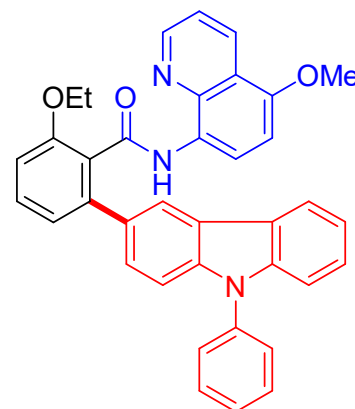
9d: $\lambda_{\text{max}} = 242 \text{ nm}$



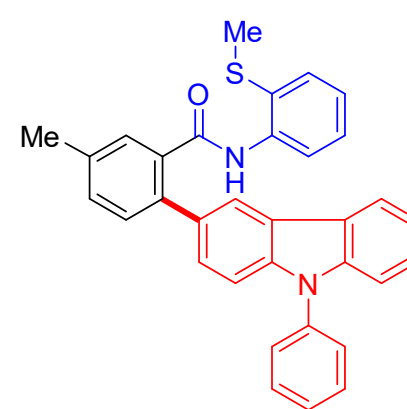
7a: λ_{max} = 244 nm



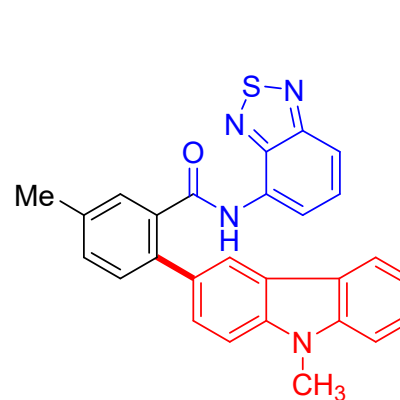
7b: λ_{max} = 241 nm



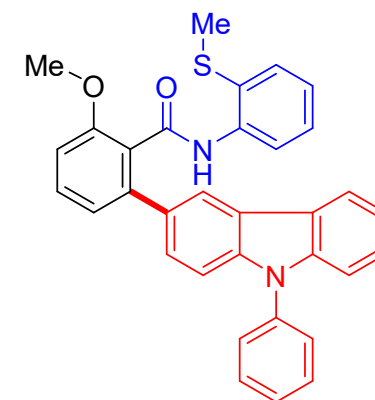
7c: λ_{max} = 249 nm



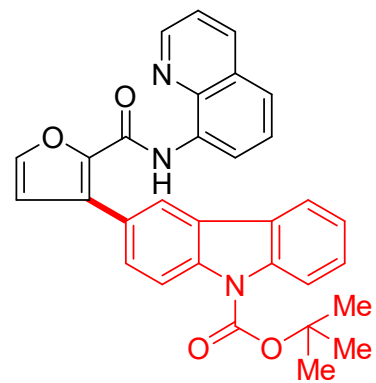
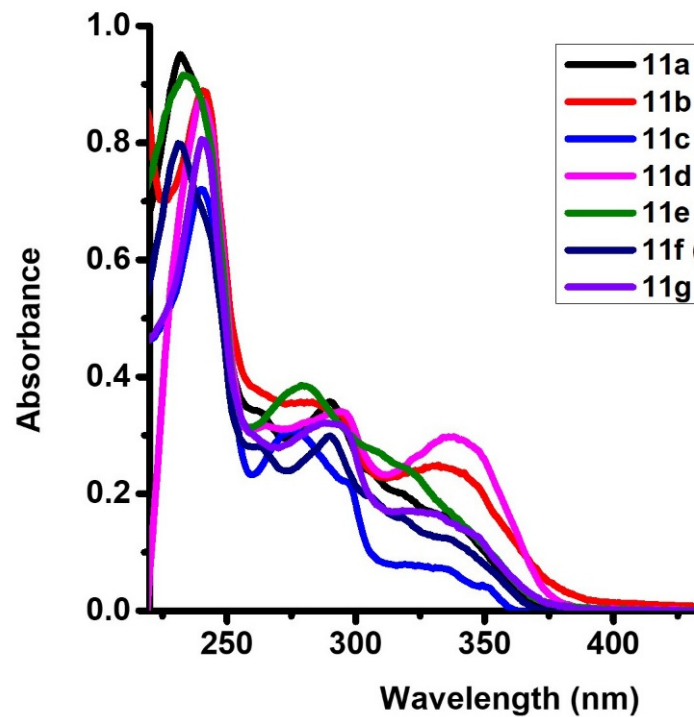
7d: λ_{max} = 247 nm



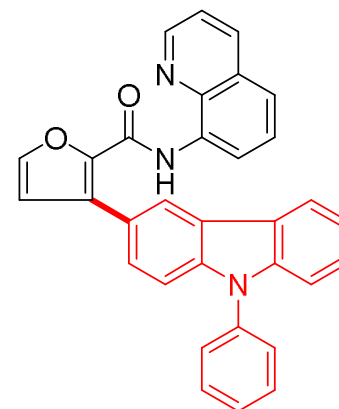
7e: λ_{max} = 239 nm



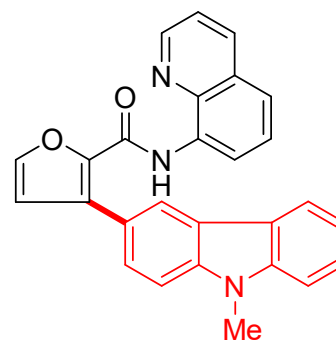
7f: λ_{max} = 245 nm



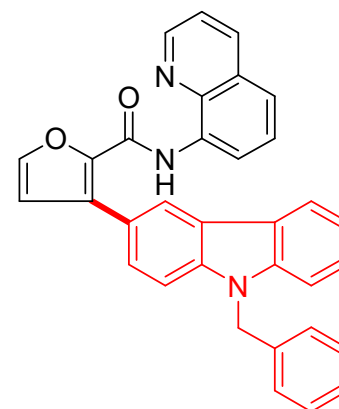
11a: $\lambda_{\text{max}} = 232 \text{ nm}$



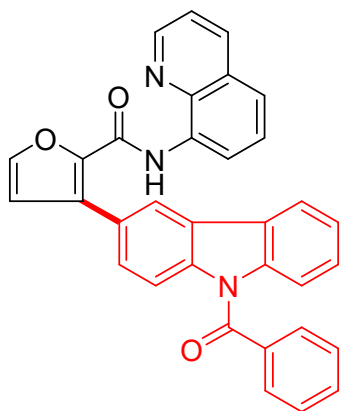
11b: $\lambda_{\text{max}} = 242 \text{ nm}$



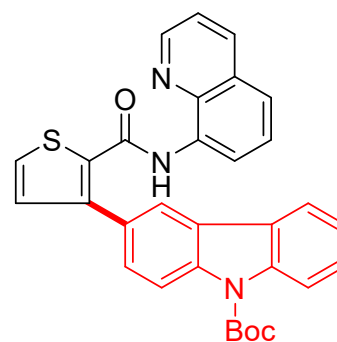
11c: $\lambda_{\text{max}} = 240 \text{ nm}$



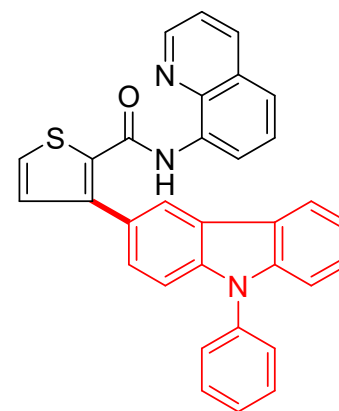
11d: $\lambda_{\text{max}} = 241 \text{ nm}$



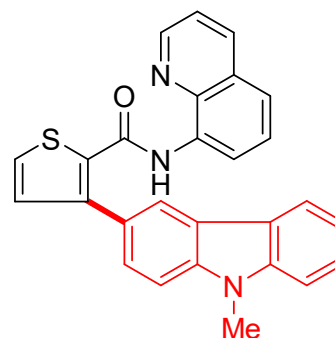
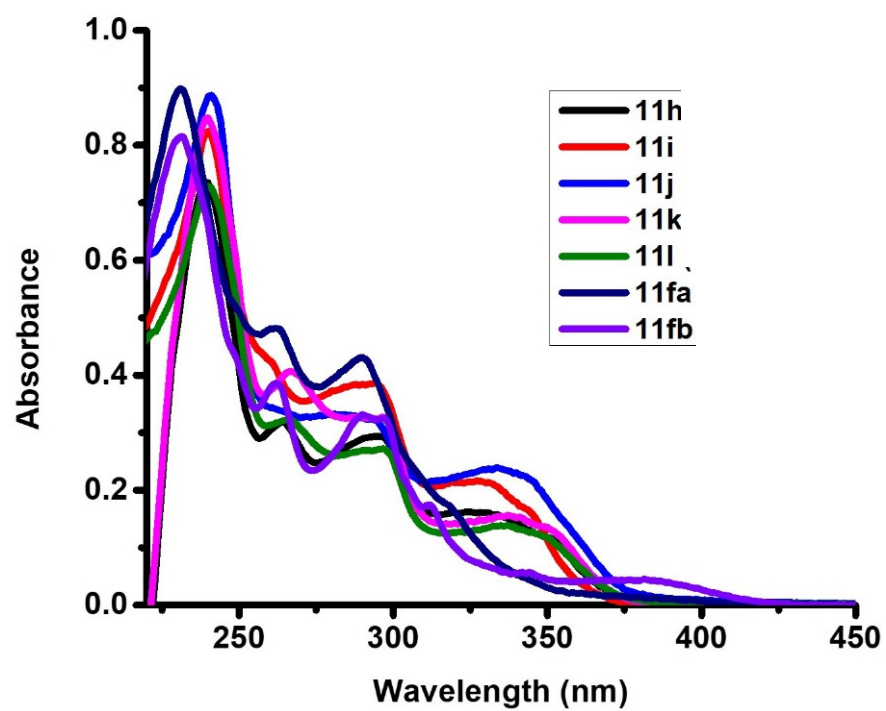
11e: $\lambda_{\text{max}} = 234 \text{ nm}$



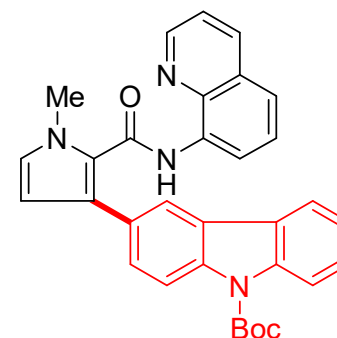
11f: $\lambda_{\text{max}} = 232 \text{ nm}$



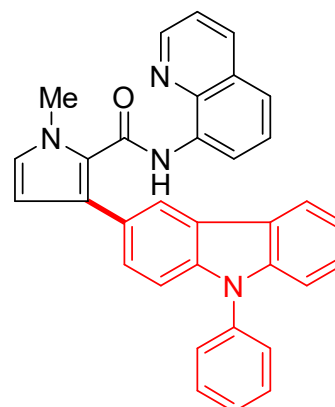
11g: $\lambda_{\text{max}} = 241 \text{ nm}$



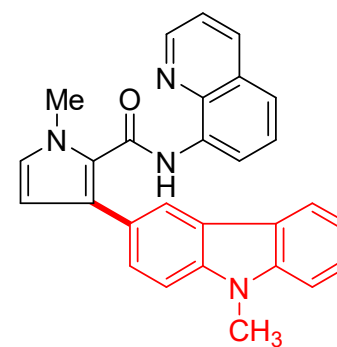
11h: $\lambda_{\text{max}} = 240 \text{ nm}$



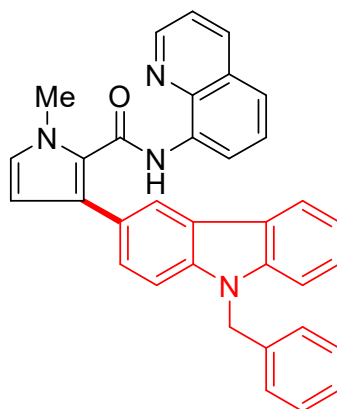
11i: $\lambda_{\text{max}} = 240 \text{ nm}$



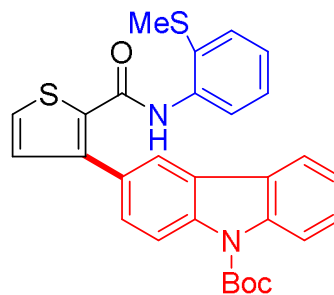
11j: $\lambda_{\text{max}} = 240 \text{ nm}$



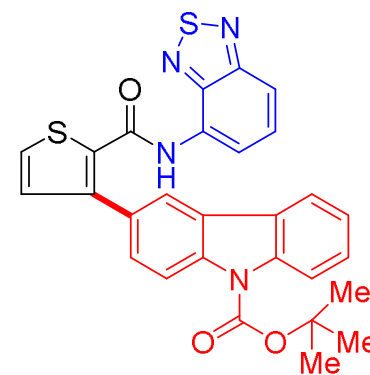
11k: $\lambda_{\text{max}} = 240 \text{ nm}$



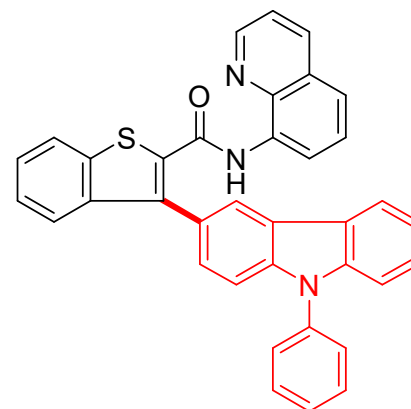
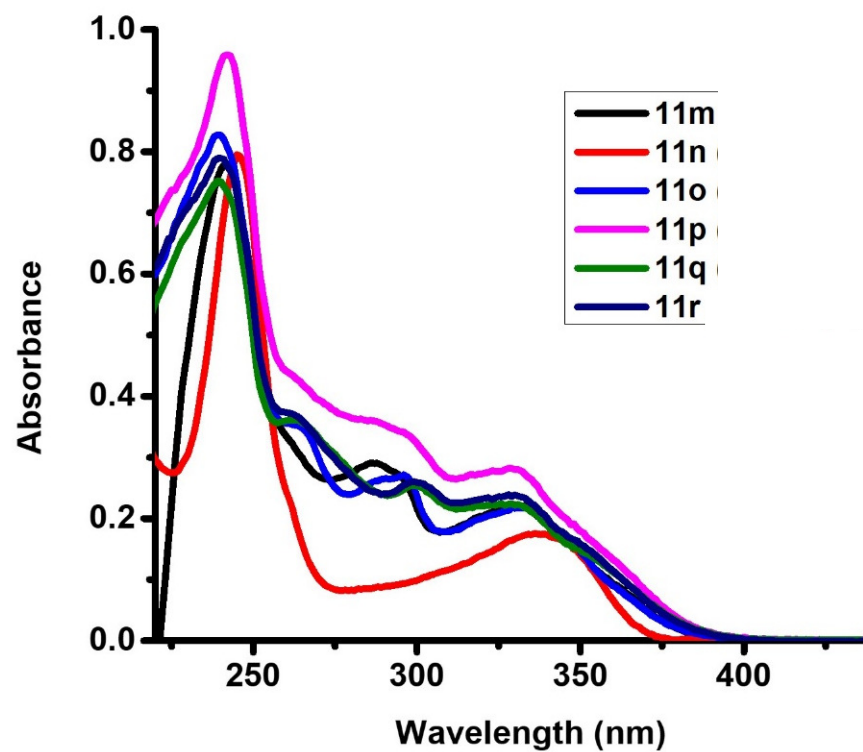
11l: $\lambda_{\text{max}} = 240 \text{ nm}$



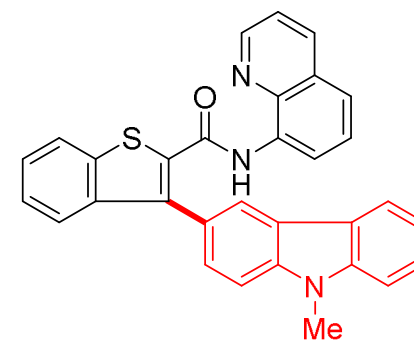
11fa: $\lambda_{\text{max}} = 231 \text{ nm}$



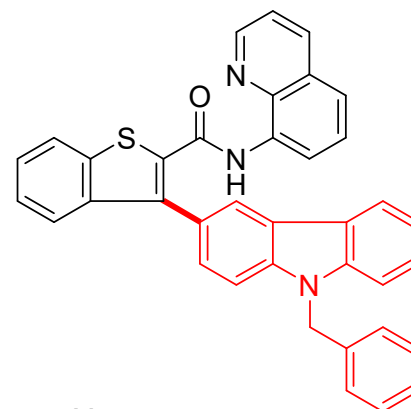
11fb: $\lambda_{\text{max}} = 232 \text{ nm}$



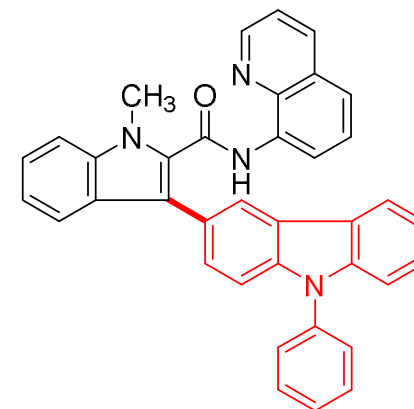
11m: $\lambda_{\text{max}} = 241 \text{ nm}$



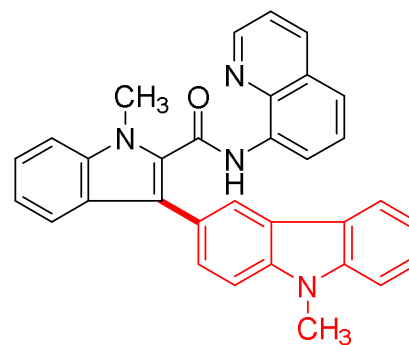
11n: $\lambda_{\text{max}} = 246 \text{ nm}$



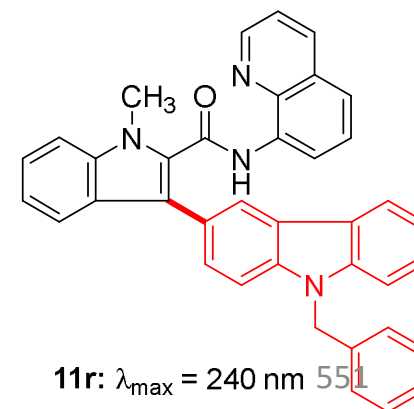
11o: $\lambda_{\text{max}} = 240 \text{ nm}$



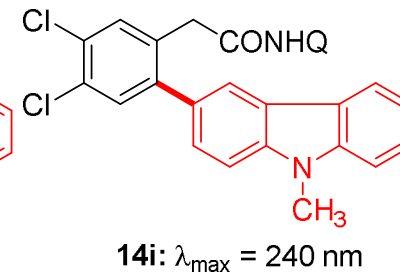
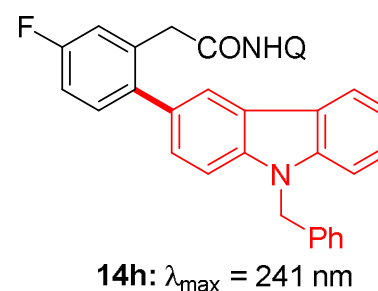
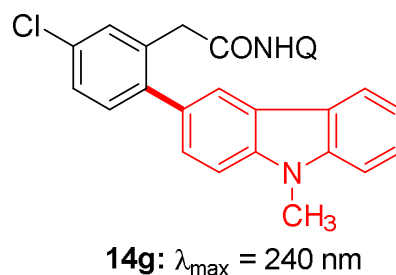
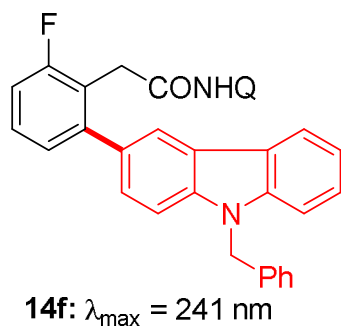
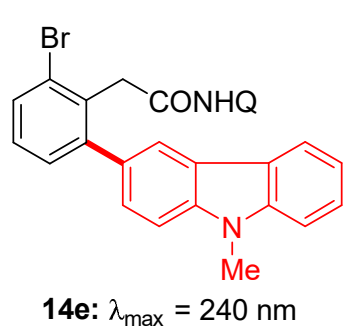
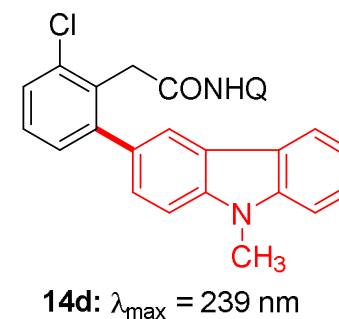
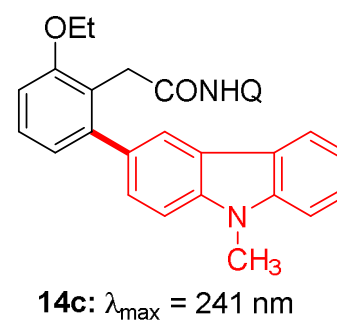
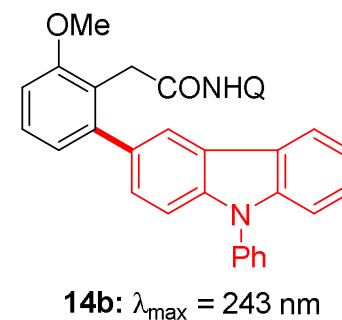
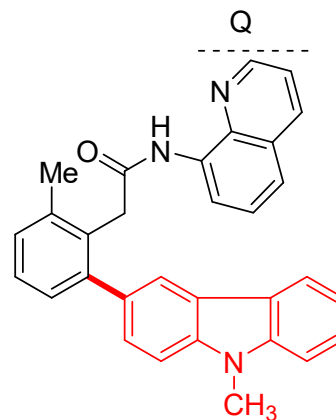
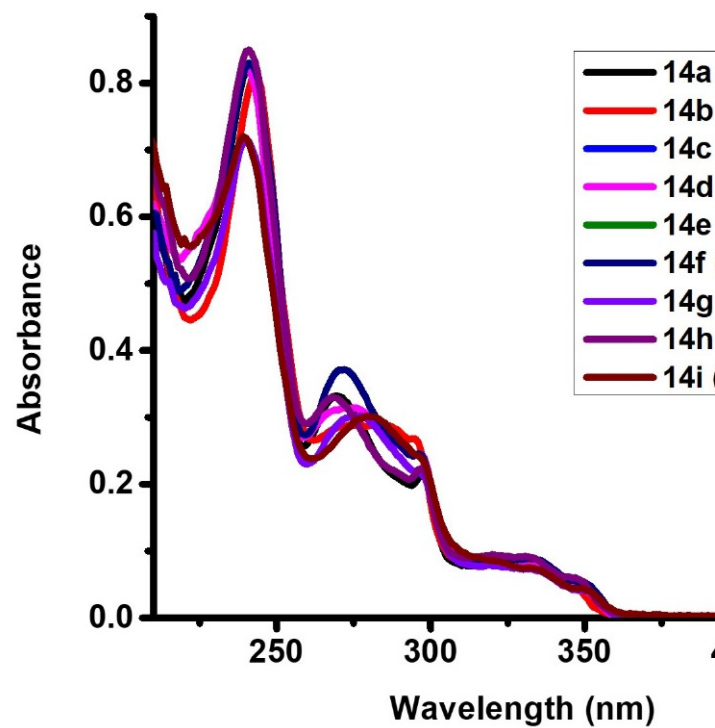
11p: $\lambda_{\text{max}} = 242 \text{ nm}$

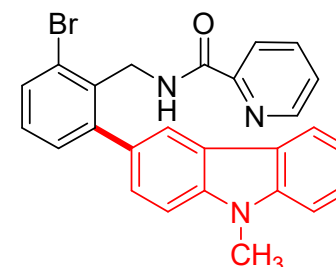
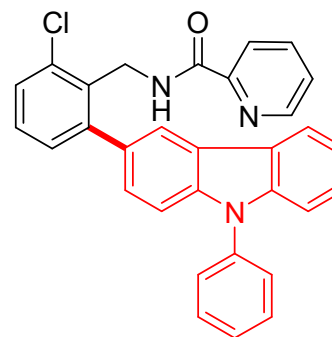
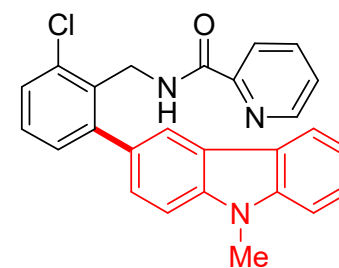
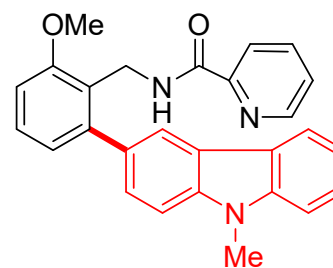
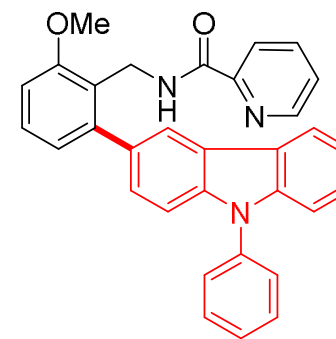
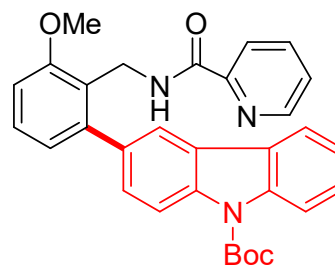
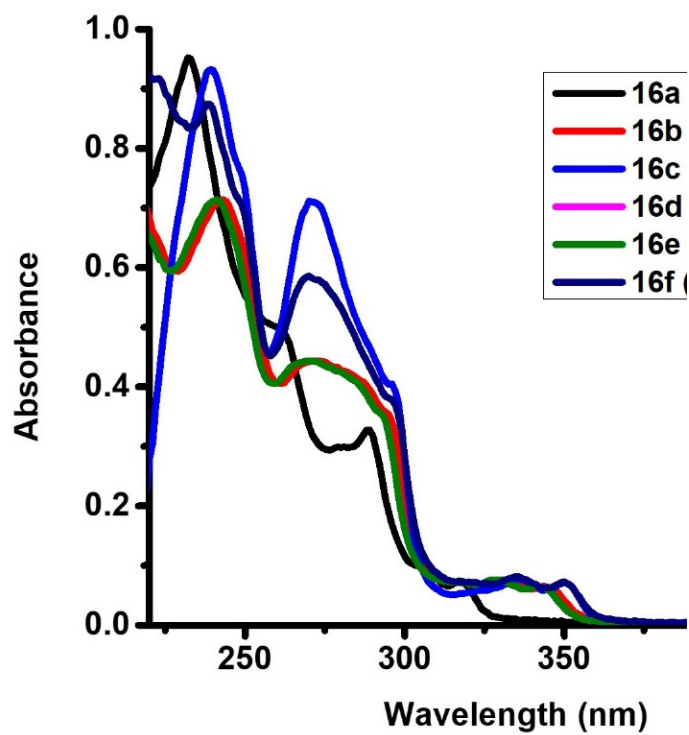


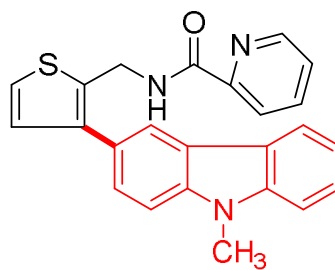
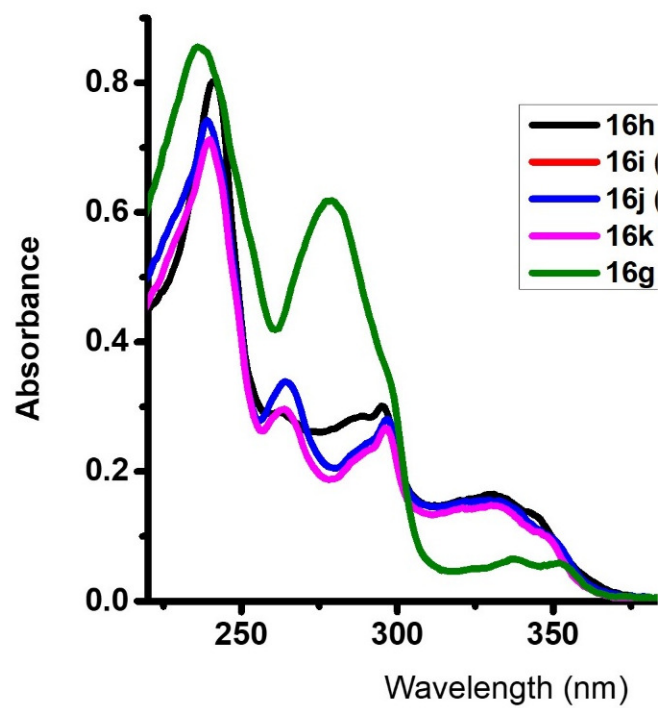
11q: $\lambda_{\text{max}} = 240 \text{ nm}$



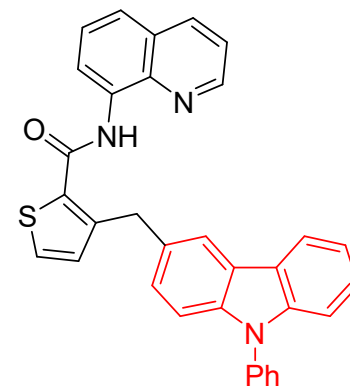
11r: $\lambda_{\text{max}} = 240 \text{ nm}$



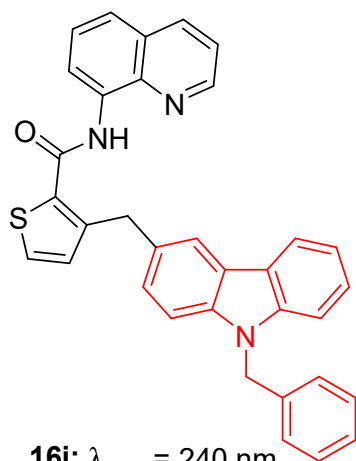




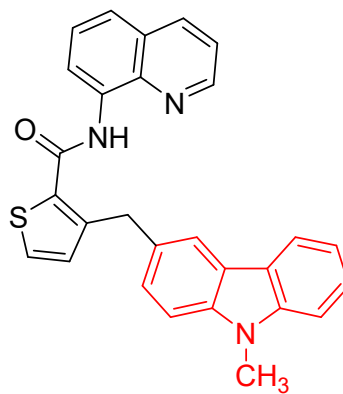
16g: $\lambda_{\text{max}} = 237 \text{ nm}$



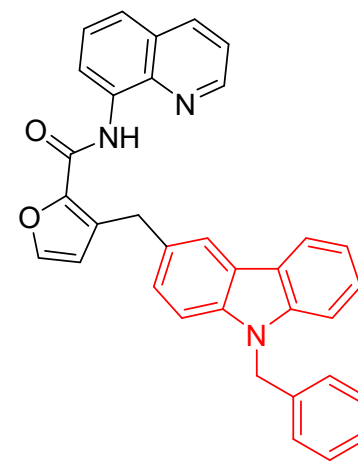
16h: $\lambda_{\text{max}} = 242 \text{ nm}$



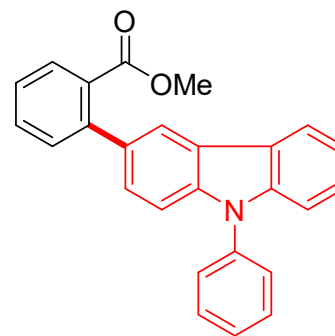
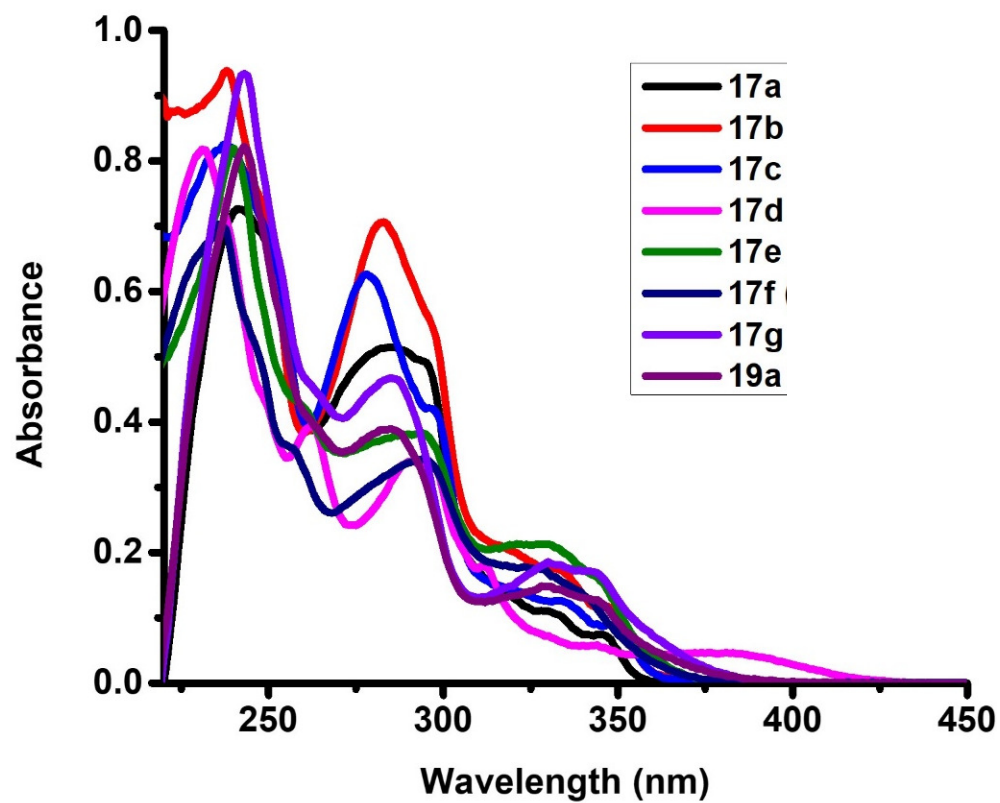
16i: $\lambda_{\text{max}} = 240 \text{ nm}$



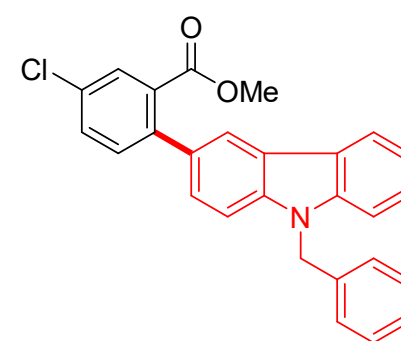
16j: $\lambda_{\text{max}} = 239 \text{ nm}$



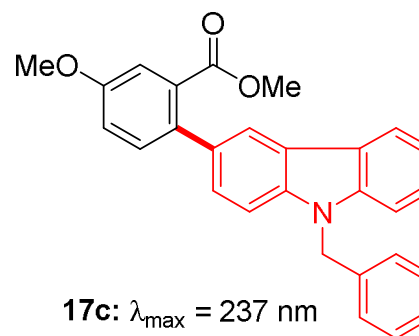
16k: $\lambda_{\text{max}} = 240 \text{ nm}$



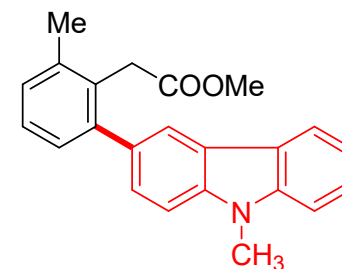
17a: $\lambda_{\text{max}} = 243 \text{ nm}$



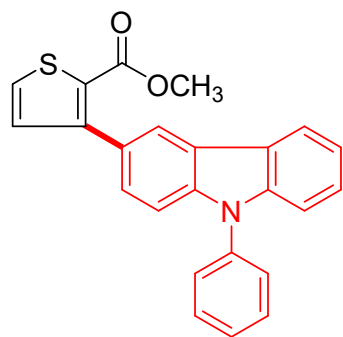
17b: $\lambda_{\text{max}} = 238 \text{ nm}$



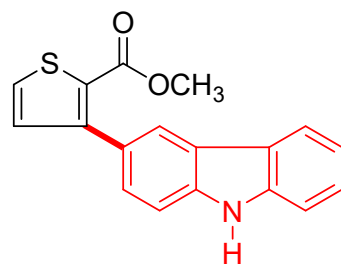
17c: $\lambda_{\text{max}} = 237 \text{ nm}$



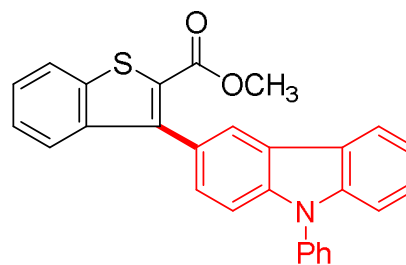
17d: $\lambda_{\text{max}} = 232 \text{ nm}$



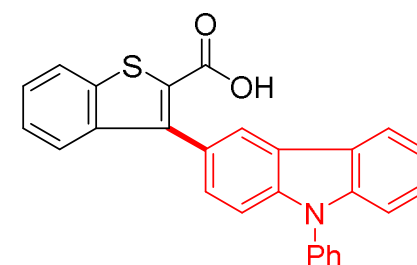
17e: $\lambda_{\text{max}} = 240 \text{ nm}$



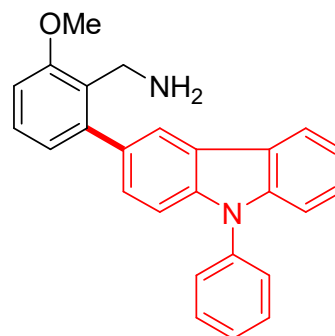
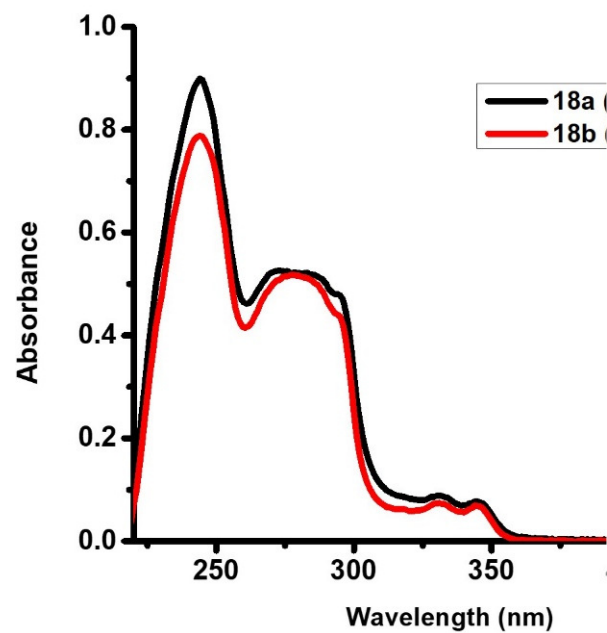
17f: $\lambda_{\text{max}} = 236 \text{ nm}$



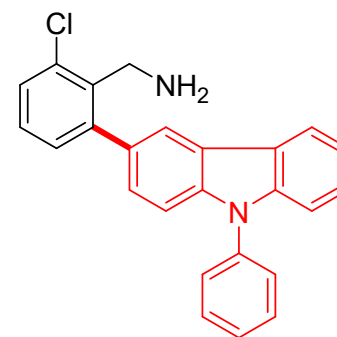
17g: $\lambda_{\text{max}} = 243 \text{ nm}$



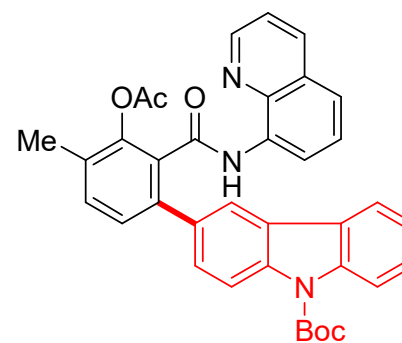
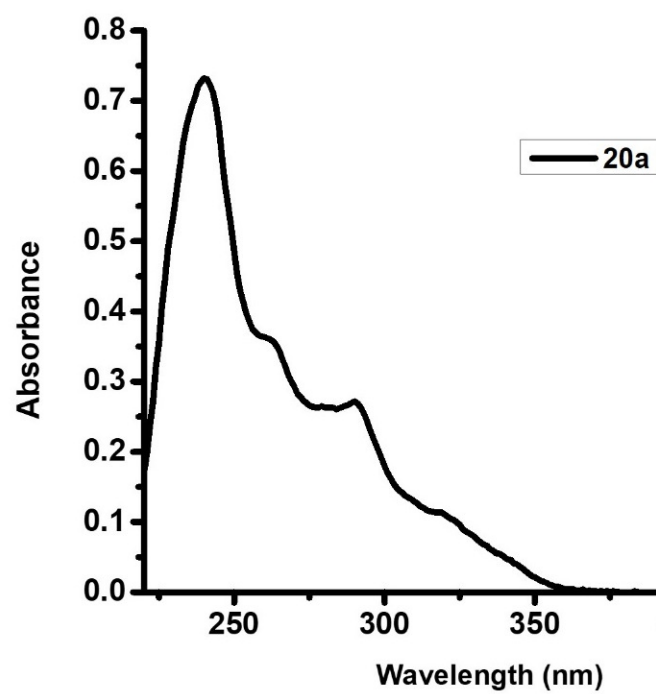
19a: $\lambda_{\text{max}} = 243 \text{ nm}$



18a: $\lambda_{\text{max}} = 243$ nm

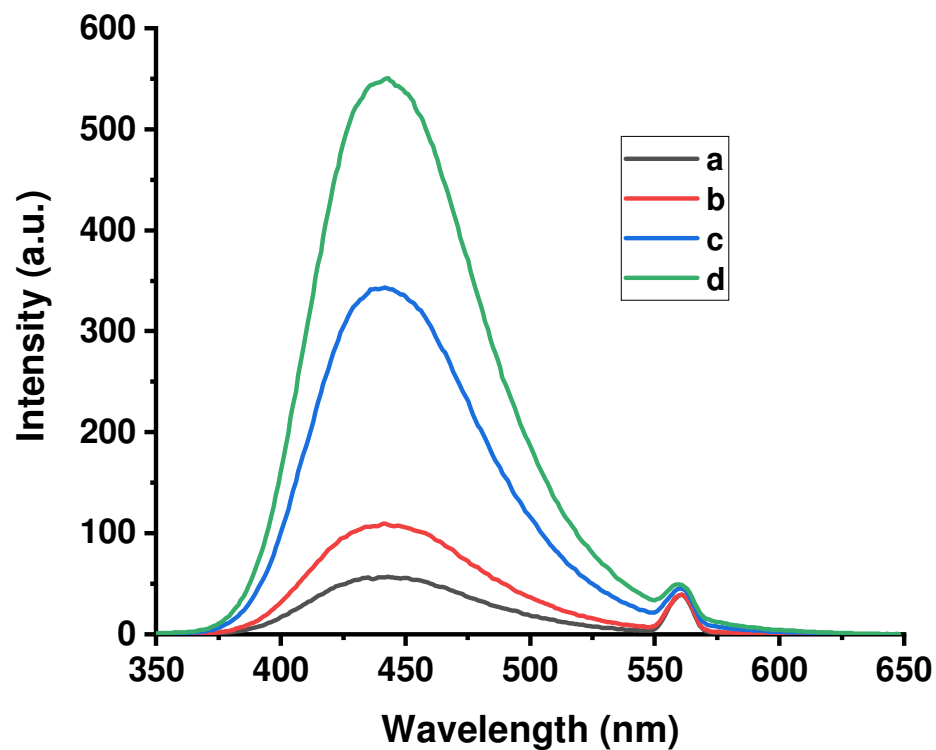


18b: $\lambda_{\text{max}} = 243$ nm



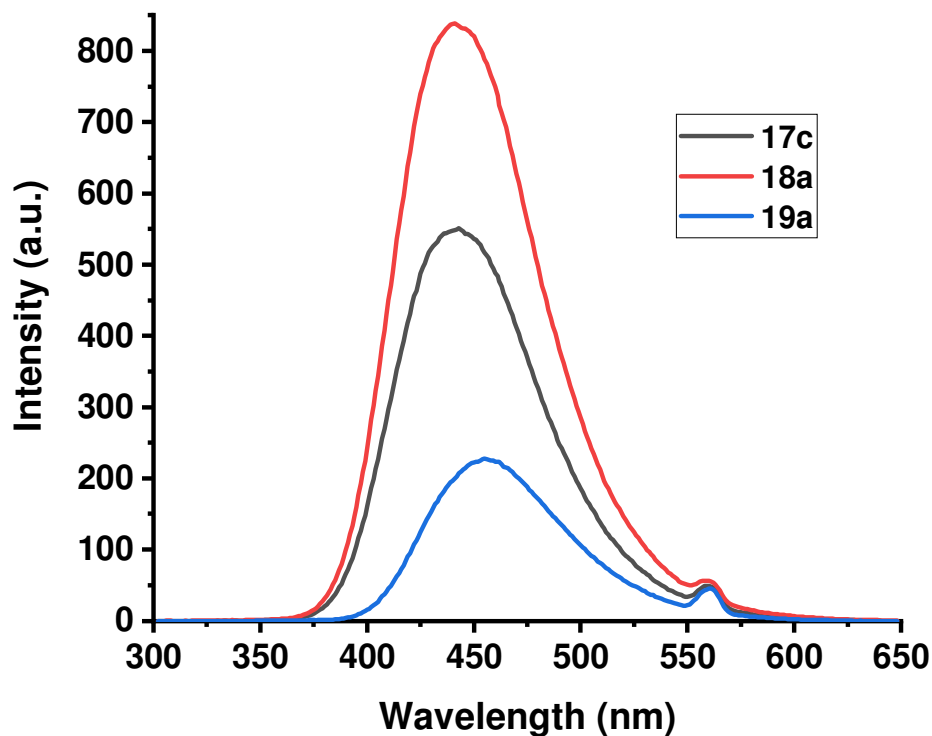
20a: $\lambda_{\text{max}} = 240$ nm

Plot 1: Emission spectra of **17c** in MeCN at 280 nm with the different concentration of sample solution.



Concentration = **a**: 0.71 μM , **b**: 1.42 μM , **c**: 4.2 μM , **d**: 7.1 μM .

Plot 2: Plot of emission spectra of **17c**, **18a**, **19a** in MeCN at 280 nm. The concentration of all the sample solutions is 7.1 μM .

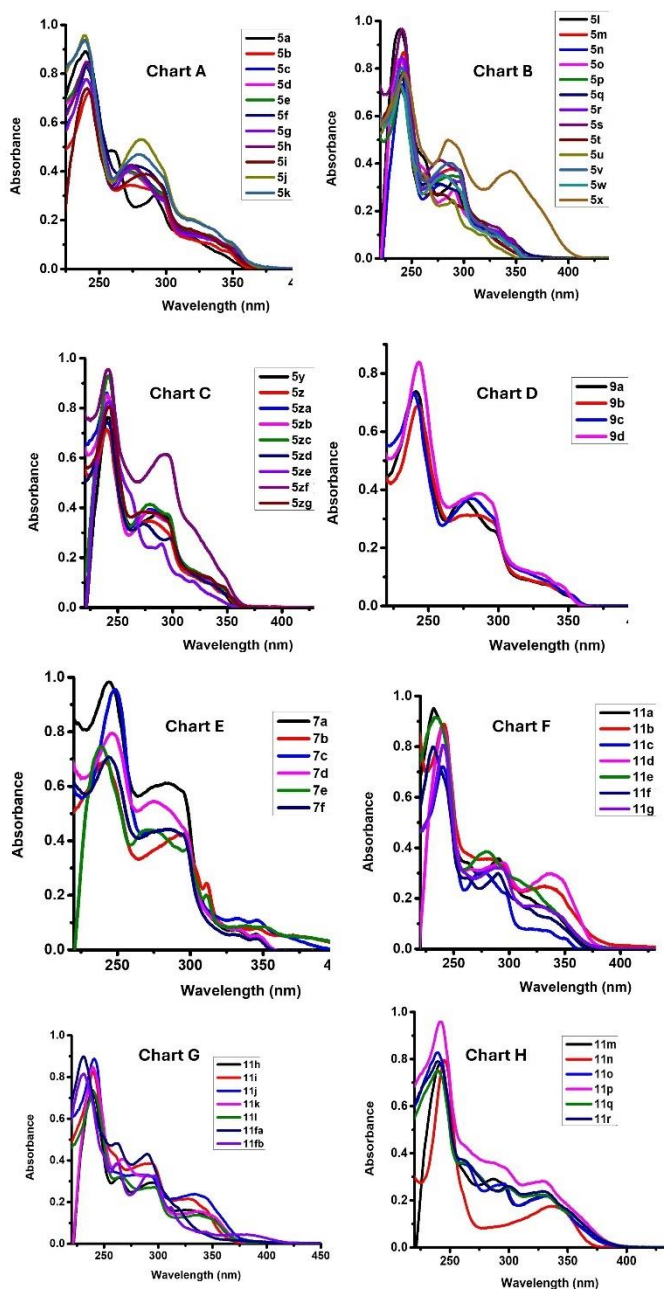


λ_{max} (emission) (nm) at the excitation wavelength of 280 nm = **17c**: 443, **18a**: 441, **19a**: 445.

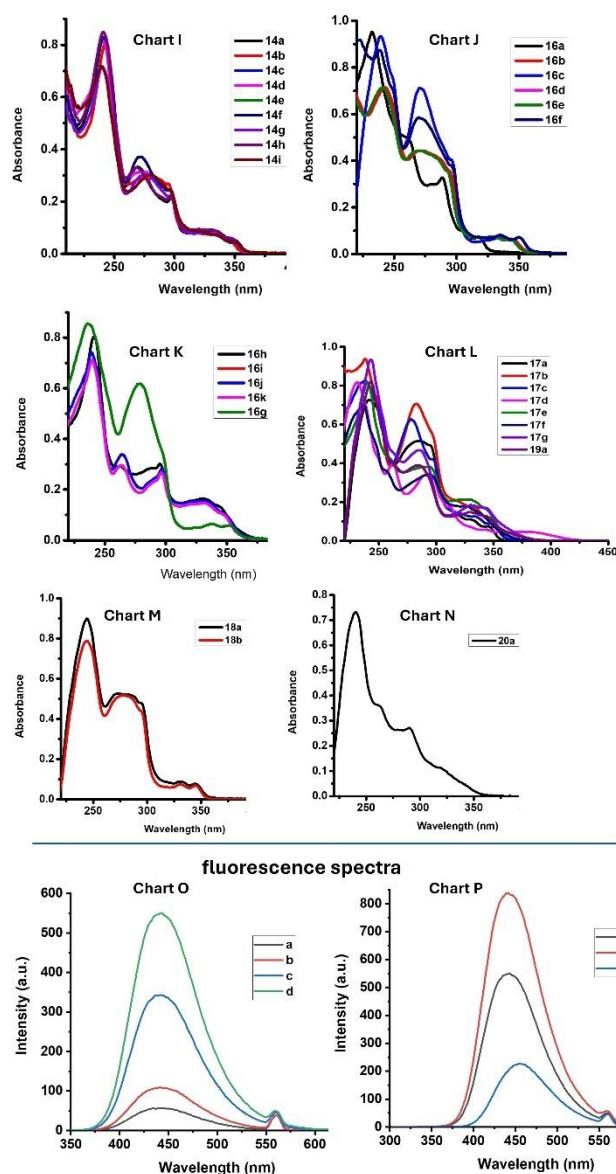
UV-Vis absorption ($\lambda_{\max}$ (nm)) and emission spectral details of compounds.

Taking an impetus from the general observations that carbazoles are fluorescent compounds and have found several applications, we have obtained the UV-Vis absorption spectra ($\lambda_{\max}$ (absorption)) of all compounds given below in Charts A to N.

UV-Vis absorption ($\lambda_{\max}$ (nm)) value for compounds, **5a** = 240, **7a** = 244, **7b** = 241, **7c** = 249, **7d** = 247, **7e** = 239, **7f** = 245, **5b** = 242, **5c** = 240, **5d** = 241, **5e** = 241, **5f** = 242, **5g** = 241, **5h** = 241, **5i** = 241, **5j** = 239, **5k** = 239, **5l** = 239, **5m** = 243, **5n** = 241, **5o** = 238, **5p** = 243, **5q** = 240, **5r** = 241, **5s** = 240, **5t** = 240, **5u** = 240, **5v** = 240, **5w** = 239, **5x** = 243, **5y** = 241, **5z** = 240, **5za** = 248, **5zb** = 241, **5zc** = 242, **5zd** = 240, **5ze** = 242, **5zf** = 242, **5zg** = 242, **9a** = 242, **9b** = 242, **9c** = 240, **9d** = 242, **11a** = 232, **11b** = 242, **11c** = 240, **11d** = 241, **11e** = 234, **11f** = 232, **11g** = 241, **11h** = 240, **11i** = 240, **11j** = 240, **11k** = 240, **11l** = 240, **11m** = 241, **11n** = 246, **11o** = 240, **11p** = 242, **11q** = 240, **11r** = 240, **11fa** = 231, **11fb** = 232, **14a** = 241, **14b** = 243, **14c** = 241, **14d** = 239, **14e** = 240, **14f** = 241, **14g** = 240, **14h** = 241, **14i** = 240, **16a** = 233, **16b** = 245, **16c** = 240, **16d** = 243, **16e** = 243, **16f** = 239, **16g** = 237, **16h** = 242, **16i** = 240, **16j** = 239, **16k** = 240, **17a** = 243, **17b** = 238, **17c** = 237, **17d** = 232, **17e** = 240, **17f** = 236, **17g** = 243, **18a** = 243, **18b** = 243, **19a** = 243, **20a** = 240.



The plot of absorption spectra of compounds, $\lambda_{\max}$ (absorption) [Charts A-H] (for all cases, the concentration of the solution was 0.01 g/100 mL in CH_3CN).

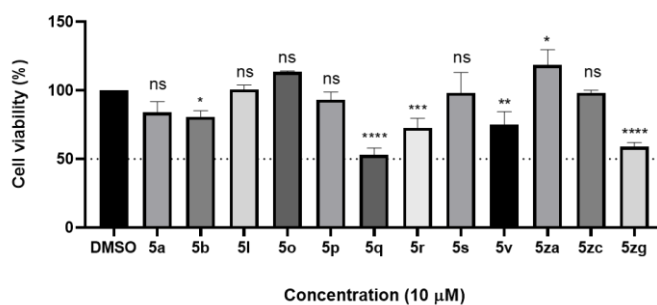


The plot of absorption spectra of compounds, λ_{max} (absorption) [Charts I-N] (for all cases, the concentration of the solution was 0.01 g/100 mL in CH_3CN). (Chart O) = Emission spectra of **17c** in MeCN at 280 nm with the different concentration of sample solution (Concentration = a: 0.71 μM , b: 1.42 μM , c: 4.2 μM , d: 7.1 μM). [Chart P] = Plot of emission spectra of **17c**, **18a**, and **19a** in MeCN at 280 nm (the concentration of all the sample solutions is 7.1 μM). λ_{max} (emission) (nm) at the excitation wavelength of 280 nm = **17c**: 443, **18a**: 441, **19a**: 445.

We have done a preliminary analysis of fluorescence emission of representative biaryl-based carbazole (Charts O and P). The Charts O is the emission spectra of **17c** in MeCN at 280 nm recorded using the concentrations of 0.71, 1.42, 4.2, and 7.1 μM , respectively. These emission spectra implied that with a relative increase in the concentration of **17c** in MeCN, the intensity of the emission is increasing, and no intermolecular interaction or quenching is occurring. We observed the emission peaks λ_{max} (emission) (nm) at the excitation wavelength of 280 nm for **17c** = 443, **18a** = 441, and **19a** = 445.

Preliminary screening of anticancer activities compounds.

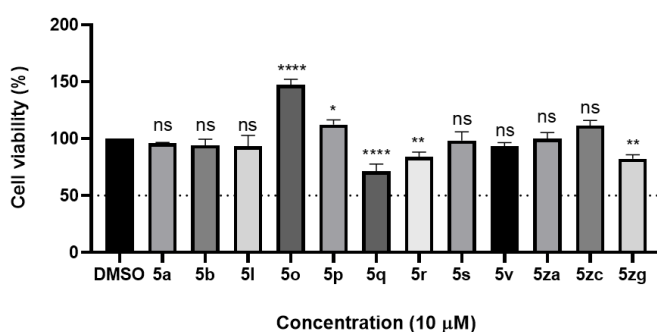
Preliminary screening - HeLa_{48 h}



****p < 0.0001, **p < 0.01, *p < 0.05

a.

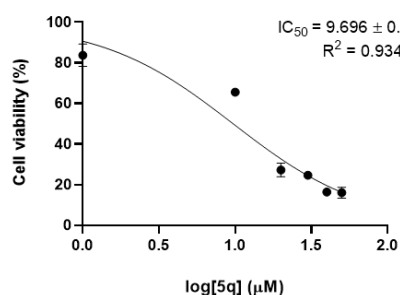
Preliminary screening - HCT116_{48 h}



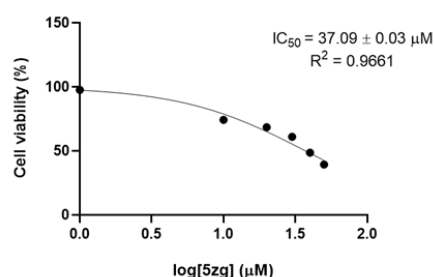
****p < 0.0001, **p < 0.01, *p < 0.05

b.

5q - HeLa

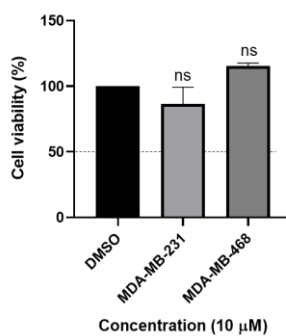


5zg - HeLa



c.

5q - Preliminary screening

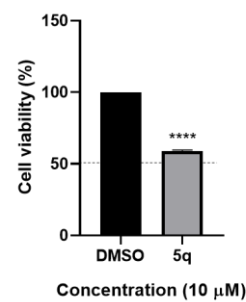


****p < 0.0001, **p < 0.01, *p < 0.05

e.

HEK293T

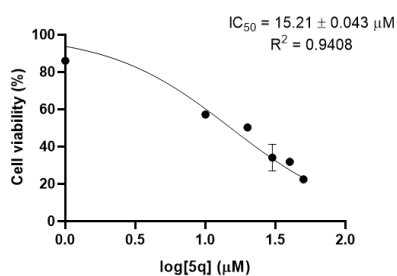
5q - Preliminary screening



****p < 0.0001, **p < 0.01, *p < 0.05

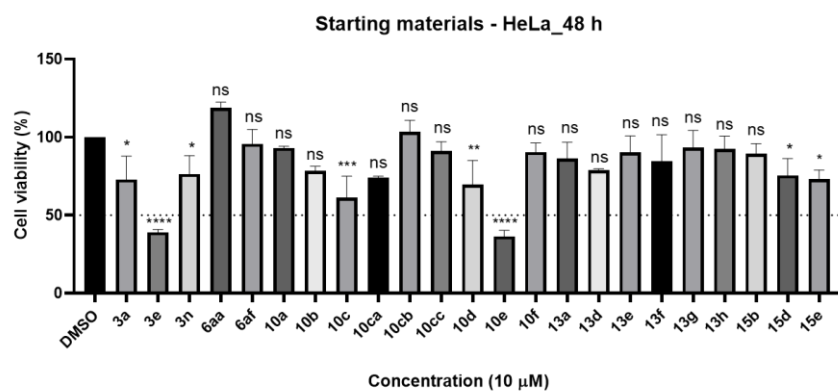
f.

5q - HCT116



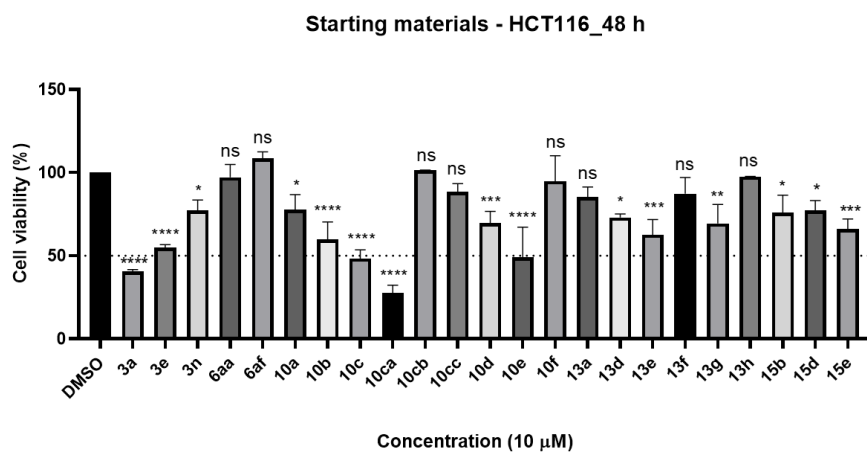
d.

Figures 1 and 2 (in manuscript). Preliminary screening and dose response of compounds 5a, 5b, 5l, 5o, 5p, 5q, 5r, 5s, 5v, 5za, 5zc and 5zg in various cell lines.



****p < 0.0001, **p<0.01, *p<0.05

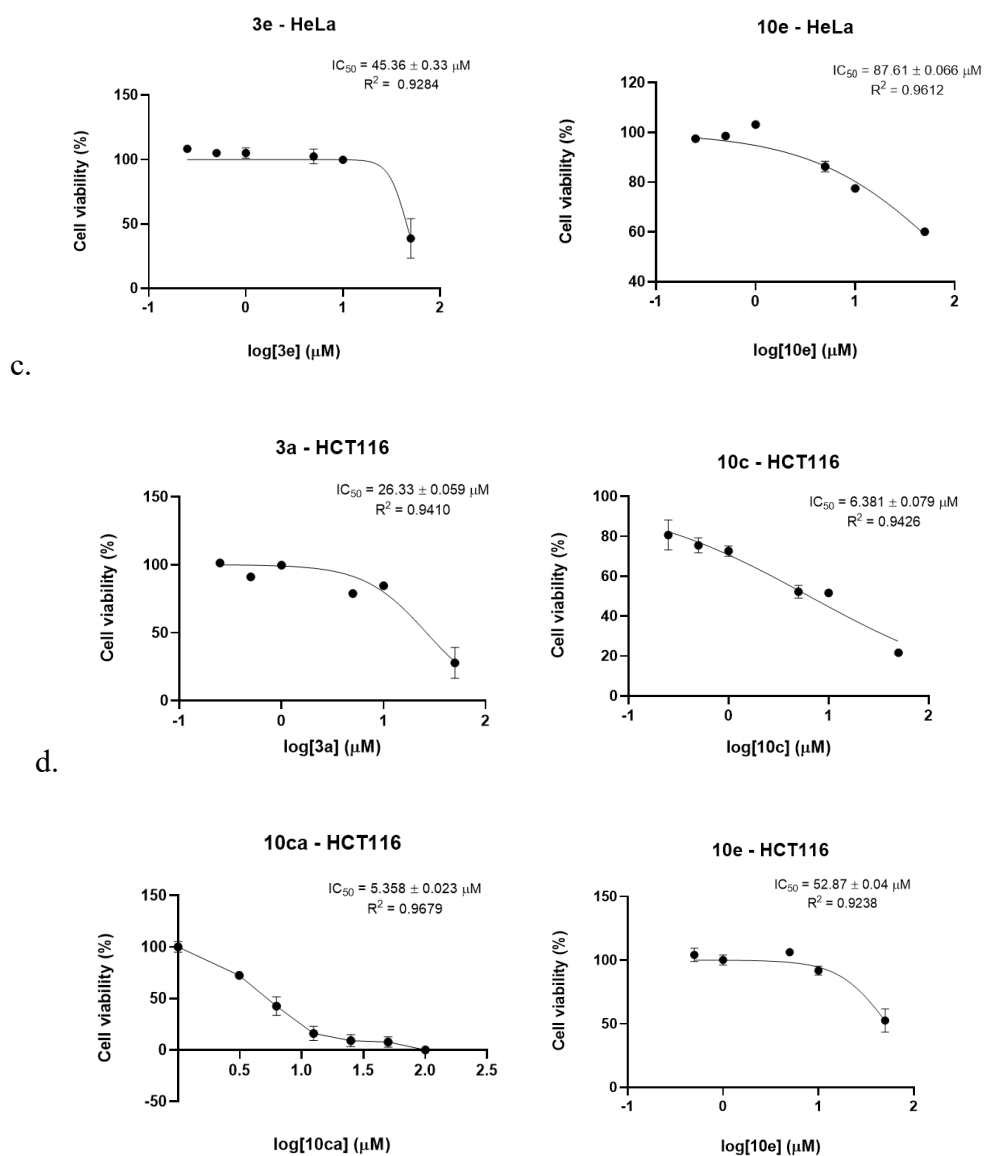
a.



****p < 0.0001, **p<0.01, *p<0.05

b.

Figure 4 (in manuscript). Preliminary screening and dose response of starting materials in HeLa and HCT 116 cell lines.



Figures 4 and 5 (in manuscript). Preliminary screening and dose response of starting materials in HeLa and HCT 116 cell lines.

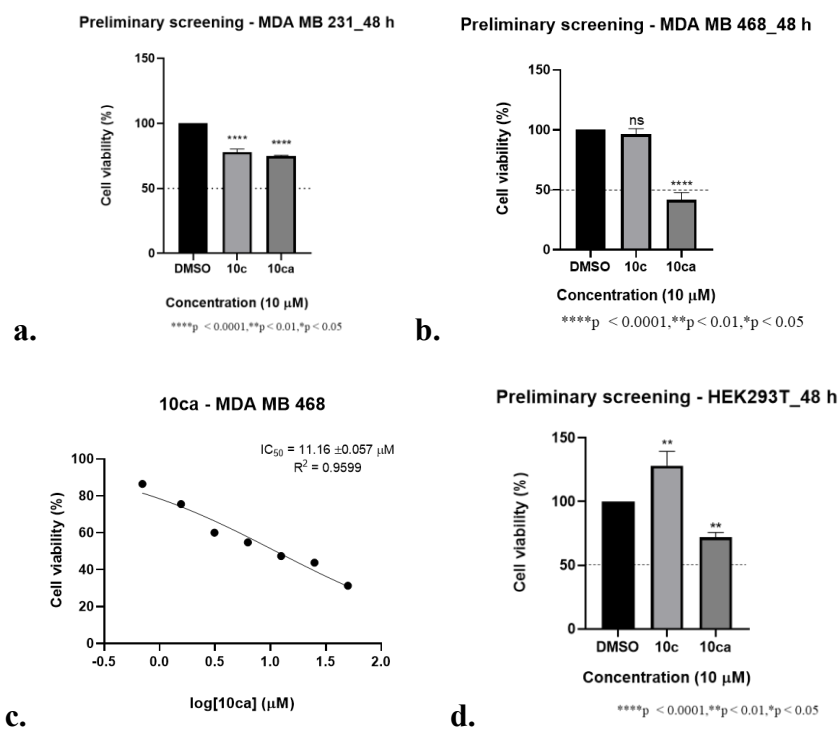
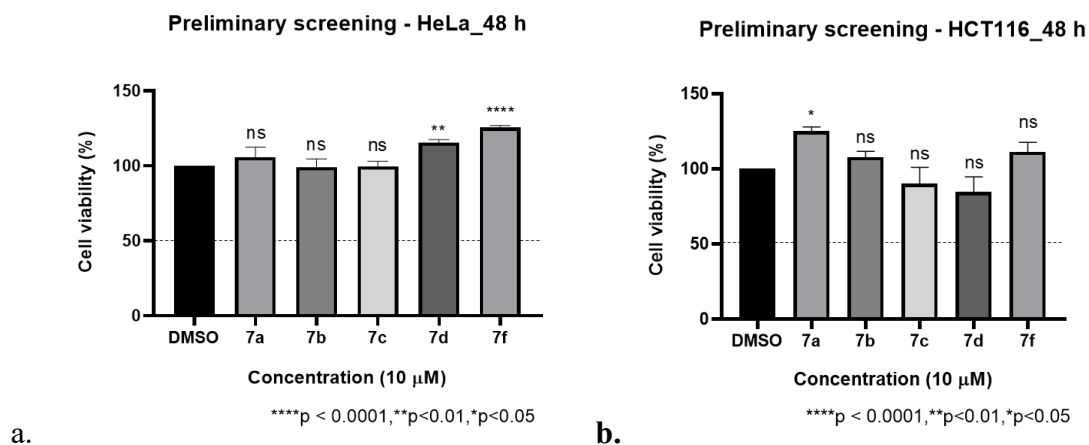
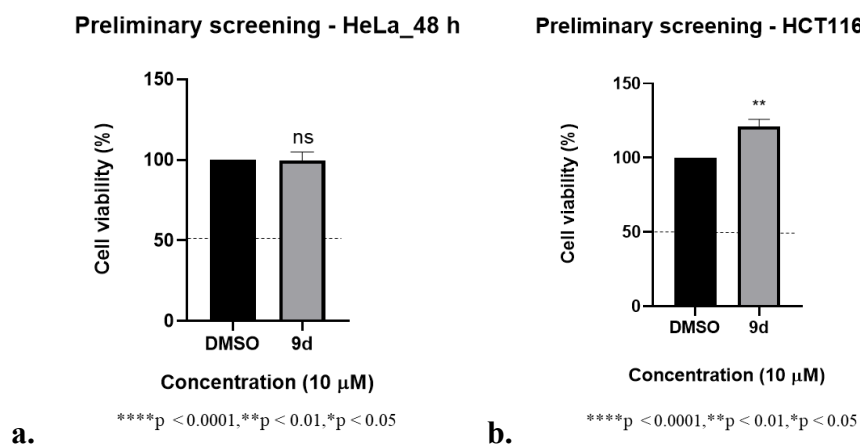


Figure 6 (in manuscript). Preliminary screening and dose response of hit starting materials in MDA-MB-231, MDA-MB-468 and HEK293T cell lines.



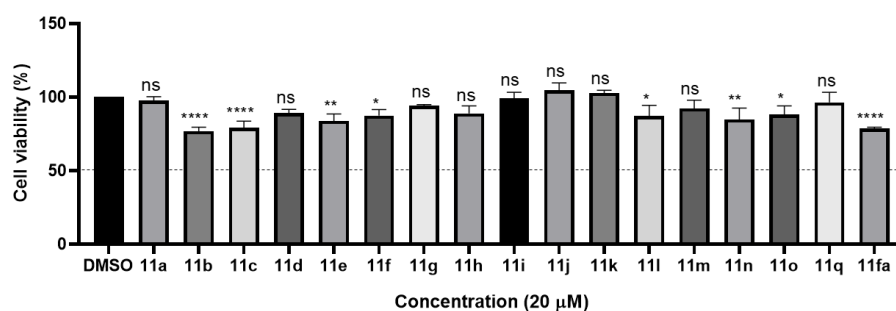
Preliminary screening of compounds **7a-f** in HeLa and HCT 116 cell lines.



Preliminary screening of compound **9d** in HeLa and HCT 116 cell lines.

Figure S1. Preliminary screening of compounds **7a-d**, **7f**, **9d**, in HeLa and HCT 116 cell lines.

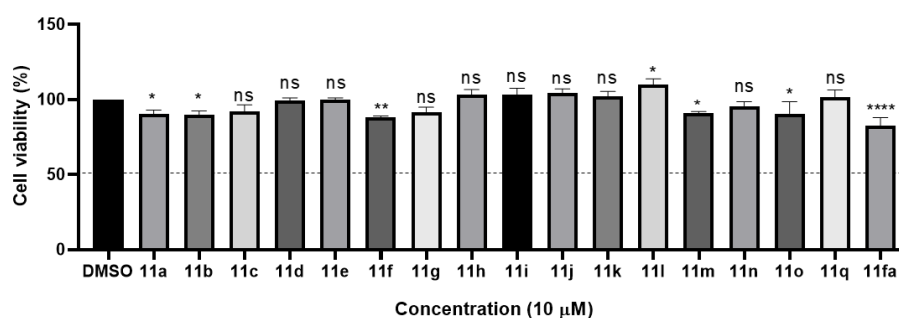
Preliminary screening - HeLa_{48 h}



a.

****p < 0.0001, **p < 0.01, *p < 0.05

Preliminary screening - HCT116_{48 h}

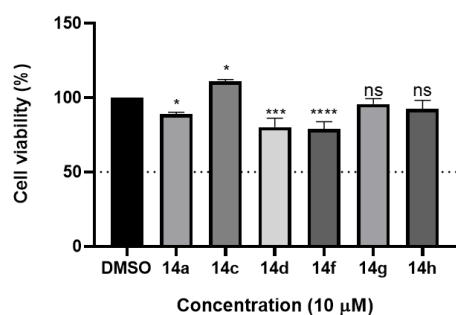


b.

****p < 0.0001, **p < 0.01, *p < 0.05

Preliminary screening of compounds **11a-o**, **11q** and **11fa** in HeLa and HCT 116 cell lines.

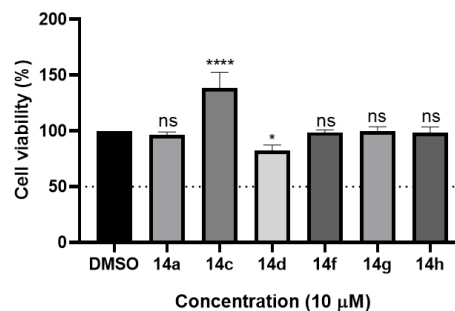
Preliminary screening - HeLa_{48 h}



a.

****p < 0.0001, **p < 0.01, *p < 0.05

Preliminary screening - HCT116_{48 h}

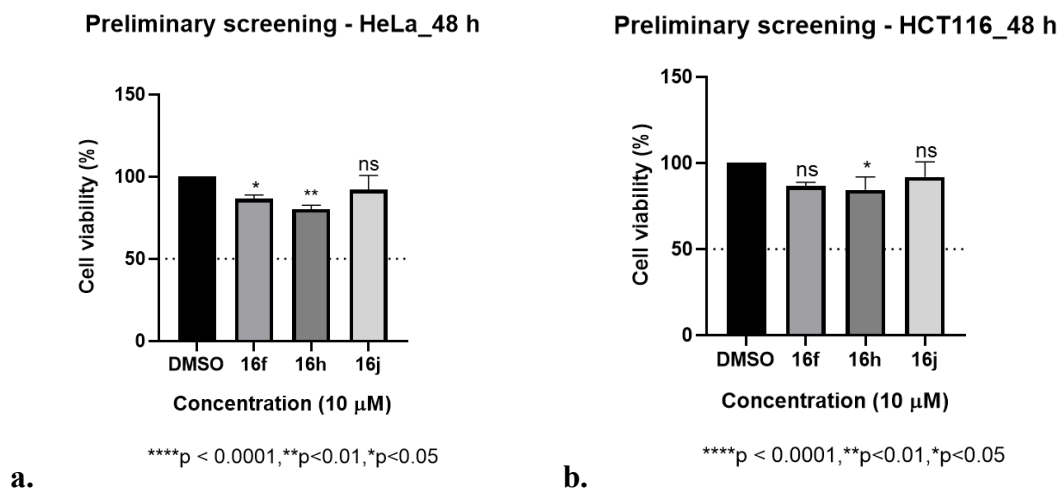


b.

****p < 0.0001, **p < 0.01, *p < 0.05

Preliminary screening of compounds **14a**, **14c**, **14d**, **14f**, **14g** and **14h** in HeLa and HCT 116 cell lines.

Figure S2. Preliminary screening of compounds **11a-o**, **11q** and **11fa**, **14a**, **14c**, **14d**, **14f**, **14g** and **14h** in HeLa and HCT 116 cell lines.



Preliminary screening of compounds **16f**, **16h** and **16j** in HeLa and HCT 116 cell lines.

Figure S3. Preliminary screening of compounds **16f**, **16h** and **16j** in HeLa and HCT 116 cell lines.